NATURAL BOUNDARY CONDITION METHODS FOR NUCLEAR REACTIONS

by

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To -

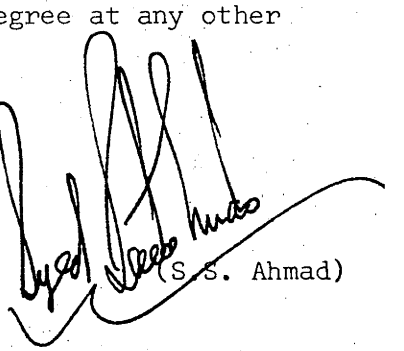
R. L. L.

STATEMENT

The author has collaborated with his supervisor, Dr B.A. Robson, in developing the IRM (Iterative *R*-matrix) method which is being reported with the BD (Barrett and Delsanto) method in Chapter 3 of this thesis. The two methods were applied to the $^{12}C(n, n)^{12}C$ reaction (Chapter 4) and the coupled square well problem (Chapter 5) in close collaboration with Dr R.F. Barrett and Dr B.A. Robson and have been reported in two publications[1,2].

The author has independently applied the IRM method to the $^{12}C(p, p)^{12}C$ reaction (Chapter 6) and some of the preliminary results were presented at the last AINSE conference[3].

No part of this thesis has been presented for a degree at any other university.



(S.S. Ahmad)

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1) S.S. Ahmad, R.F. Barrett and B.A. Robson, "Natural boundary condition methods for nuclear reactions", *Nucl. Phys.* A257 (1976) 378.

2) S.S. Ahmad, R.F. Barrett and B.A. Robson, "Natural boundary condition methods for nuclear reactions II", *Nucl. Phys.* A270 (1976) 1.

3) S.S. Ahmad and B.A. Robson, "Application of an *R*-matrix method with natural boundary conditions to $^{12}C(p, p')^{12}C$ ", unpublished, presented at Sixth AINSE Conference, University of Melbourne, 1976.

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ABSTRACT

The BD (Barrett and Delsanto) and IRM (Iterative *R*-matrix) methods for calculating cross sections are discussed. Both methods are characterized by their use of natural boundary conditions at the surfaces separating internal and external regions of configuration space and the employment of energy-dependent basis states. An energy correction which greatly improves the rate of convergence of the BD method is also given.

The methods are compared with both standard and generalized *R*-matrix calculations with energy-independent basis states for the reaction $^{12}C(n, n)^{12}C$ at incident energies below the inelastic threshold using a weak vibrational model. The convergence of the natural boundary condition methods was found to be substantially better than for the other cases. Moreover, the methods are used to calculate both the elastic and inelastic scattering cross sections for an exactly soluble model comprising two square well potentials coupled by a square well interaction. The methods are investigated for weak, intermediate and strong coupling interactions and the results are compared where possible with those of other related methods. It is concluded that for the practical calculation of reaction cross sections from a basic physical model, the natural boundary condition methods offer the most tractable approach particularly for problems involving strong channel coupling.

The IRM method is also applied to the $^{12}C(p, p)^{12}C$ reaction below 8 MeV using a collective rotational model for the target nucleus. The predictions of the method are again substantially better than the standard *R*-matrix method and are in good agreement with the equivalent coupled-channels calculations.

CONTENTS

CHAPTER 1

INTRODUCTION

The various stages in the development of the theory of nuclear reactions incorporating resonance phenomena seem to resemble very much the following pattern which appears to be followed by most physical theories that have taken a considerable period to develop:

(i) Evolution of a "hypothesis" from the available experimental and related theoretical evidence.

(ii) Translation of the hypothesis into a rigorous "mathematical language".

(iii) Identification of the "transient" and "inherent" characteristics of the physical formulation.

(iv) Reorganization of the inherent characteristics in the form of a "theory" which enables one to describe the physical phenomenon in a logically coherent and mathematically consistent way.

(v) Deduction of the basic physical content of the theory from very general principles by other alternative "methods".

(vi) Search for the "best" amongst all the available methods so that the physical phenomenon can be explained in the framework of the most rational theoretical approach.

The occurrence of sharp resonances in the total scattering cross section was pointed out about forty years ago in connection with the systematic *experimental studies* of a variety of low-energy nuclear reactions[1-9]. Since then a tremendous amount of accurate experimental data on low- and intermediate-energy resonances has been accumulated. Throughout this period the theorists' interests were to understand the underlying resonance mechanism and to incorporate it in the framework of a sound and

coherently formulated reaction theory.

In analogy with the "compound molecule" approach employed for the interpretation of a few chemical reactions[10], the first successful attempt on these grounds was the "compound nucleus" hypothesis of Bohr, Breit and Wigner[11-15]. Accordingly, a reaction process may be considered as being the succession of two causal events. The first is the union of the projectile and target particles to form a relatively long-lived compound nucleus having well defined virtual energy levels. The second event is the disintegration of this compound system into final product. Thus the resonances observed in the total reaction cross sections can be described in terms of a rapid sharing of the projectile's (kinetic) energy among all the target constituents. The importance of this hypothesis lies in the fact that it is still regarded as a basic postulate of many reaction theories.

The compound nucleus *hypothesis was simultaneously translated into a reasonable mathematical language* i.e. the Breit-Wigner formula[13] for calculating the resonance cross sections proceeding via an intermediate state. Based upon a development analogous to the time-dependent perturbation theory employed for the emission and absorption of optical radiations, the formula gave satisfactory fits to the isolated resonances observed in several nuclear reactions[16,17]. However, apart from its success, the underlying assumptions were open to criticism and have been widely discussed in the literature[18-24]. It is perhaps worth emphasizing that by taking into account both the failures and the successes of the Breit-Wigner formalism, theorists[25-29] were able to *identify the inherent as well as the general characteristics* necessary for the foundation of a reasonable reaction theory.

The *reorganization* of these initial efforts in understanding the mechanism of nuclear resonance reactions led eventually to the development of two well defined theories of nuclear reactions: the Kapur-Peierls

theory[30,31] and the *R*-matrix theory of Wigner and Eisenbud[32-34]. The basic idea of the Kapur-Peierls theory is that the configuration space of all the interacting nucleons may be regarded as a black box type "internal" region surrounded by an "external" region. Being independent of either any perturbation treatment or the detailed dynamics of the system under consideration, the theory employs a set of eigenstates in the expansion of the wave function for the internal region. These eigenstates are matched at the "surface" connecting the two regions by imposing purely outgoing wave "boundary conditions" which causes the eigenvalues and all other parameters to be complex and implicitly energy-dependent. Consequently, apart from its rigorous mathematical framework, the theory has not been pursued much further for practical applications. However, some recent calculations[35,36] have indicated that if carefully employed, the theory may reflect some meaningful aspects of the resonance phenomena.

Using a similar division of configuration space, Wigner[17,21,32-34] developed the *R*-matrix theory which gave a general approach for the practical calculation of resonant as well as non-resonant cross sections. Starting from the Schrödinger equation for the interacting system, the theory simply assumes that there exists a solvable Hamiltonian which can completely specify the state of the system in the external region. On the other hand, the Hamiltonian for the internal region may be too complicated to solve, either because of the unknown nuclear forces or due to the lack of knowledge regarding the exact behaviour of the compound system. The merit of the *R*-matrix theory is that the value of the wave function on the surface can be related to the corresponding normal derivatives there through a definite quantity; the *R*-matrix. The latter may be parametrized in terms of the available experimental data so that an overall estimate of the cross section can be obtained from the corresponding unitary and symmetric scattering matrix.

The Kapur-Peierls and Wigner-Eisenbud theories employ distinct mathematical techniques and emphasize different aspects of resonance behaviour. They seem to have led to the foundation of the so-called "structural" and "dynamical" approaches for the theoretical description of resonance phenomena. The former[37-42] deals with a perspicuous parametrization of the resonant cross sections but may be inapt when a detailed study of the overall scattering (reaction) process is desired. The latter, on the other hand, introduces the nuclear dynamics by incorporating a suitable (phenomenological or microscopic) nuclear model and hence enables one to perform actual calculations for a complete description of the reaction processes. The reason why dynamical approaches have been more appreciated seems to emerge from the fact that during the last three decades the well known nuclear models[43-46] (i.e. Shell models and collective models) have substantially contributed to the epistemology regarding the nuclear interior. Thus it appears quite natural to use an appropriate nuclear model which can predict the salient features about the dynamics of the compound system and thereby extract more physical parameters for using in the reaction theory.

Soon after the development of the *R*-matrix theory and its application to many nuclear problems, there was *increasing interest in deducing the general physical content of a theory of resonance reactions from different viewpoints* necessary for the particular requirements of nuclear, atomic and molecular physics. Such an enthusiasm has given rise to an exceedingly large number of theories or formal methods for treating various scattering processes. Lane and Robson[48-52] have successfully discussed almost all of these methods in a comprehensive manner by setting up a formal framework incorporating the earlier attempts due to Bloch[53,54].

Despite the fact that numerous reaction theories have provided definite mathematical frameworks for determining the cross sections from a given model Hamiltonian, there has not been much effort in *crystallizing the best*

amongst them. This is mainly due to the inadequate one-to-one correspondence between any theoretical formulation and its proper numerical application to particular reactions. However, the advent of extremely sophisticated computers has enhanced the study of these theories on the basis of actual realistic calculations. Such studies[55-75] have been very useful in providing a "numerical test" by virtue of which one may not only determine the extent to which a formulation is accurate but also methods of improving it.

In this respect the coupled-channels formulation has been quite promising irrespective of the fact that a straightforward solution of the problem requires a given set of coupled integro-differential equations which may be very cumbersome to solve in some practical cases. However, since its formulation by Bohr and Mottelson[76] together with the suggestions of Feshbach[77-79] and the success of optical model[80] analyses, the method has been employed considerably for analysing the elastic and inelastic scattering of light particles from collective nuclei[66,70,81-89]. Although the coupled-channels formulation is capable of producing satisfactory fits to many data, it is difficult to incorporate the exchange, rearrangement and breakup processes[90] and to include the antisymmetrization of the target and incident particle in a straightforward manner. Hence, apart from these difficulties, the method is suitable to use as a reference for checking and further development of other formal theories.

As stated earlier, the *R*-matrix theory of Wigner and Eisenbud[18,32-34] is one of the better known approaches for relating the nuclear scattering and reaction cross sections to the underlying nuclear dynamics[42]. Thus, in recent years there has been increasing interest in applying the valuable experience and relevant ideas of the *R*-matrix theory for achieving the ambitious goal of developing a method which is more accurate, widely applicable, numerically fast and needs a minimum of the computer core for storage. Hence, starting from a critical analysis of the *R*-matrix theory

and the related existing methods (e.g. the standard R-matrix method[47], the generalized R-matrix method[48-50,58,59,75], the Buttle corrected R-matrix method[63], the variationally corrected R-matrix method[91,92] and the eigenchannel method[93-96]), the main purpose of the present work is to discuss two new methods (the so-called natural boundary condition methods) and investigate how these methods improve further the present status of formulations involving the R-matrix theory for describing the scattering and reactions in the resonant and non-resonant regions.

The starting point of all these methods is the standard R-matrix (SRM) method[47] in which the nuclear wave function in the internal region is expanded in terms of a set of orthonormal eigenfunctions of the nuclear Hamiltonian which satisfy energy-independent and real homogeneous boundary conditions at the surfaces separating the two regions of configuration space. In principle, the boundary conditions are arbitrary and the results are independent of the choice of basis states. For practical purposes, however, it is necessary to truncate the infinite series by considering only a finite set of basis states. This approximation is the most crucial assumption of the SRM method because the nuclear wave function and hence the corresponding R-matrix elements usually incorporate only a small part of the infinite sums. Furthermore, in order to achieve a desirable accuracy, the number of terms in the series is often required to be large.

In view of the flexibility in the choice of boundary conditions and size of the internal region, one way of circumventing this defect of the SRM method is the employment of the generalized or extended R-matrix (GRM) method based on the ideas propounded by Tobocman and Nagarajan[58] and further developed by Lane and Robson[48-52]. The method deals with basis states which satisfy so-called "inhomogeneous" boundary conditions at the matching radii and are "non-orthogonal" over the internal region. However,

some detailed calculations[75] incorporating the set of harmonic oscillator states have shown that the method requires a significant number of basis states per reaction channel and appears to be only semiconvergent. Furthermore, for a given set of channel radii, the range in the number of basis states required for satisfactory convergence seems to be rather restricted so that some care is required to ascertain that the results are acceptable. The situation may be improved further by employing a criterion proposed by Philpott and George[75] for choosing the best set of channel radii. However, the necessary radii can only be found by an iteration procedure and in general will depend upon the incident energy.

Alternatively, instead of the boundary condition parameters and channel radii, the unsatisfactory convergence of the SRM method can be due to the neglect of the remaining terms in the infinite series. In order to account for this deficiency, Buttle has suggested an efficient correction[63] to the SRM method. The development of the concepts involved in this correction may become transparent by considering a simple structural analysis of the exact (infinite dimensional) Hilbert space spanned by the eigenfunctions of the nuclear Hamiltonian within the internal region. The SRM method employs only the "near" (truncated) part of this space whereas the Buttle corrected *R*-matrix (BCRM) method saturates the complete space with the assumption, however, that all states in the "remaining" (distant) space are uncoupled. This is the reason why, even though working with an infinite basis set and yielding improved results, the Buttle correction becomes less effective when the coupling to and between the states in the distant space becomes important.

The immediate logical improvement to the BCRM method should, therefore, be a formulation which takes a complete account of the variation in the coupling strength between states belonging to the distant space. This is precisely the idea which has given rise to the variationally corrected *R*-matrix (VCRM) method of Zvijac, Heller and Light[92]. They employ the

Buttle corrected wave function as a trial function in the Kohn variational formula[99] to achieve a higher degree of accuracy with fewer basis states in cases where the BCRM method gives poor convergence.

Amongst all the *R*-matrix type methods, the eigenchannel (EC) method[93-96] is quite distinct in the sense that it is characterized by the explicit treatment of "all" the eigenstates (i.e. eigenchannels) and the phase shifts associated with the eigenvalues (i.e. eigenphases) of the "total" *S*-matrix for the reaction under consideration[100,101]. Moreover, in contrast to the *R*-matrix wave functions, the EC wave functions converge uniformly at the boundary of the internal region. The method has been exposed to several numerical tests employing realistic[61,64,68] as well as model[102] reaction problems in the framework of a particle-hole treatment of one-particle in continuum. It has been found that provided the coupling is not too strong, a small number of basis states is sufficient to reproduce the exact results. Moreover, the method is able to handle, at least in principle, three- and many-particle reactions and even the cluster channels[103-106].

At this stage one may ask, "what is the need of searching for more methods when there already exist such a hierarchy of *R*-matrix type methods?" The answer to this question seems to be hidden in the following statement excerpted from the pioneering work of Lane and Robson[48]: "All theories are exact, and so are equivalent if applied exactly. It is only when applied in an approximate manner that some theories may be more useful in that they give a better first approximation". It is actually *the quest for this better first approximation which has led to the development of the natural boundary condition* (NBC) *methods* which will be the main subject of the present work.

In fact the configuration mixing and resultant lack of convergence

occurring in the practical application of the SRM method is a result of the boundary condition mixing and the residual interaction which is not completely accounted for by the one-body nuclear potential. The effect of the latter may be reduced by choosing a realistic model for the central nuclear potential and the effect of the former may be minimized by an optimum choice of the boundary condition parameters. The quantitative investigations in the effect of the choice of these parameters have given rise to the formulation of two methods for calculating the reaction cross sections. Both methods are closely related in that they are based on the assertion that if the basis states obey "natural boundary conditions", the number of basis states required for the satisfactory convergence may be kept to a minimum(*). This is particularly important in nuclear as well as atomic or molecular physics where the number of reaction channels is large.

The methods differ somewhat, however, in numerical techniques. Involving the "matrix diagonalization" technique, the first method is a generalization of an approach which was suggested by Danos and Greiner[107] for the single channel case and eventually abandoned in favour of the eigenchannel method[96]. This method is essentially that of Barrett and Delsanto[108] and is much faster numerically than the eigenchannel approach. Although the method may be called a "matrix diagonalization" method[109], it will be referred to hereafter as the "Barrett and Delsanto (BD)" method. The second method is the SRM approach which employs the "matrix inversion" technique; but instead of incorporating, as is customary, a fixed set of

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(*) This point will be elaborated in connection with the appropriate definition of the natural boundary conditions in Chapter 3.

basis states for all energies, it uses an energy-dependent basis chosen by an iteration procedure based explicitly upon the fact that a finite set of basis states with natural boundary conditions provides the best estimate of the cross section. This method will be called the "Iterative *R*-matrix (IRM)" method.

Amongst the various fundamental assumptions necessary for the development of a non-relativistic treatment of low-energy reaction theories, the present work will be based on the Schrödinger picture of collision phenomena[110,111]. Only elastic- and inelastic-scattering reactions will be dealt with. Moreover, apart from an appropriate treatment of the Coulomb interaction, the interaction between the target and the projectile (or the outgoing particle and the residual nucleus) will be assumed to be negligible beyond a certain radial distance characterized by the channel radius. In general the effect of all surface or direct processes together with the channels corresponding to charge-exchange, rearrangement, breakup into three- or many-particle fragments and all the creation or absorption processes will be considered unimportant. Finally, unless otherwise stated, all central potentials involved will be assumed to be real and local; satisfying the usual fundamental principles of symmetry and invariance necessary for the employment of the Schrödinger formulation[112-115].

Starting from a brief review of the existing *R*-matrix type methods for calculating the cross sections of resonance reactions in the following chapter, the NBC methods and a convenient energy correction to the BD method, which appears to yield improved results for typical cases, will be discussed thoroughly in Chapter 3. As a first test of the success of these methods in solving realistic nuclear problems, Chapter 4 will deal with their application to the widely studied $^{12}C(n, n)^{12}C$ reaction below the inelastic threshold of 4.43 MeV employing a model Hamiltonian of Reynolds *et al*[66]. In addition, the comparison of the results with the standard and

generalized R-matrix methods together with the corresponding experiments [116-120] and coupled-channels calculations[66] will also be discussed. Furthermore, in order to investigate the numerical accuracy and the effect of correction to the BD method, Chapter 5 will be devoted to a detailed study of calculations performed in an energy region below as well as above the inelastic threshold for an exactly soluble model[121] comprising two square-well potentials coupled through a square-well. The results will be compared where possible with those from the SRM, GRM, BCRM methods and other related theories for cases of weak, intermediate and strong couplings. Finally, in Chapter 6, one of the NBC methods (i.e. IRM) will be applied to the elastic-scattering reaction of protons from ^{12}C below 8 MeV using a collective model for the ^{12}C nucleus. Again, a comparison of the results with the SRM method and the coupled-channels calculations of Mikoshiba *et al.*[70] will be used to establish the usefulness of the method for more complicated but realistic nuclear reactions.

CHAPTER 2

REVIEW OF *R*-MATRIX TYPE METHODS

2.1 Introduction

The considerable experimental knowledge accumulated so far in nuclear, molecular and atomic physics has been a consequence of the scattering data provided by detailed studies of typical collision phenomena. In nuclear physics, with which the present work will be mainly concerned, the various collision processes (i.e. elastic, inelastic, charge-exchange, stripping, pickup, breakup and photonuclear reactions) have been the major source of information about the internal structure of nuclei. In most of these data the observed cross sections consist of some narrow and/or broad resonances superimposed upon a smooth background. Thus the ultimate goal of every reaction theory should be to *predict* an accurate description of these quantities.

Although, at a first glance, the resonances may be regarded as analogues of "bound states in the continuum", it is too difficult to describe them naturally in a bound state theory. The main reason for this is the typically distinct characteristics of the operators and wave functions in the continuum region (e.g. the non-Hermiticity of the momentum operators and functions of these operators together with the intrinsically complex nature and nonuniqueness of the scattering wave functions). The usual prescription for their incorporation into a reaction theory is to expand the physical wave function in terms of some known set of discrete states. In order to fulfil these and other requirements, several reaction theories have been proposed which may be classified into the following two groups.

(A) **Structural theories:** These are the class of *S*-matrix theories which, instead of dealing with any dynamics of the system under consideration, are based on structural assumptions. Such assumptions

are the conservation of flux and time reversal invariance together with certain analytic properties of the S-matrix e.g. the existence of poles (which may be identified with the observed resonances) and the Jost functions[122,123] in the complex momentum plane.

Despite a great deal of research starting from the works of Peierls[38] and Le Couteur[39] and developed by Humblet[37,41], Rosenfeld[40] and others from various viewpoints[42,124-126]; these formulations cannot be used as a definite tool for calculating reaction cross sections. The main reason is that although these methods provide a suitable prescription for parametrizing nuclear resonances, they are incapable of establishing any definite relation to the dynamic structure of nuclei.

(B) Dynamical theories: Contrary to the structural theories, several dynamical theories have been worked out which can be applied to almost any kind of reaction process. Although it is not very easy to classify them in a strict sense, they may be identified according to the employment of any of the following artifices:

(i) modification of the boundary condition

(ii) modification of the Hamiltonian

(iii) modifications of both the boundary condition and the Hamiltonian.

The theories of class (i) are distinguished by the division of configuration space of the system, consisting of any pair of nuclei c, into an internal and an external region; separated by a hypersurface. The resonant states are specified by imposing certain boundary conditions on the eigenstates of the total Hamiltonian. Consequently, the resonances can be parametrized in terms of the characteristics of the internal region and the behaviour of these eigenstates at the surface. The theories of class (i) include the Kapur-Peierls theory[30,31], the Wigner-Eisenbud theory[18,32-34], the Brown-de Dominicis theory[127,128] and the K-matrix theory[129].

On the other hand, the theories of class (ii) take into account an explicit separation of the total Hamiltonian into a "model" and a perturbing Hamiltonian; the strength of the latter, however, being small for practical purposes. Some examples of the theories of this class are those due to Feshbach[77-79], Rodberg[130], MacDonald[131-133] and Herzenberg *et al.*[134] Although the dynamics of the whole system together with the internal motion of the target can be taken into account quite satisfactorily in these theories, practical difficulties are encountered in handling the effects of antisymmetry, the construction of appropriate projection operators and the treatment of rearrangement and breakup reactions.

Finally, the theories of class (iii) seem to emerge as a result of the assertion that "if two formulations visualize the same physical phenomena, a systematic combination of their salient features may give a new formulation which should be capable of furnishing further information about the phenomena". In view of the fact that the resulting formulations employ the basic structure of the theories in classes (i) and (ii), it seems to be more plausible to refer them as new *methods* rather than new *theories*. Starting from the "standard" and "generalized or extended" R-matrix methods[47-52,58], these new methods include the Buttle corrected R-matrix method[63], the variationally corrected R-matrix method[92], the eigenchannel method[93-96] and the natural boundary condition methods[108,109].

In this chapter an attempt will be made to discuss some of the above methods. As far as possible, the following discussion will be based on the Bloch L-operator approach[53,54,135], which has been employed extensively by Lane and Robson[48-52] and Robson and Robson[136] for developing a detailed and comprehensive formulation of several reaction theories. After giving a general discussion of the R-matrix theory in the following section, the subsequent sections will describe the standard, generalized, Buttle corrected

and variationally corrected R-matrix methods. Finally, a brief discussion regarding the present status of these methods together with a summary of the main results will be given in Section 2.6.

2.2 R-matrix theory

Consider the general two body reaction

$$x(a', z') + X(A', Z') \rightarrow [C(A, Z)] \rightarrow y(a'', z'') + Y(A'', Z'') \quad (2.2.1)$$

where a low-energy projectile (x) interacts with the target nucleus (X) to produce a compound system (C) of mass number A and charge Z which in turn gives rise to elastic, inelastic and rearrangement reactions according to the nature of the product particle (y) and the residual nucleus (Y). The 3A dimensional configuration space is divided into two distinct regions; a bounded (internal) region Ω separated by a hypersurface Λ from its complement i.e. the external region where the compound system may decay into several possible "alternatives". Each such alternative or "channel", say c, will be assumed to contain only two particles, say α_1 and α_2, having a minimum radial distance a_c; the so-called "channel radius". The hypersurface is characterized by channel radii which may, in principle, vary for different channels.

Before proceeding further, it is necessary to specify a particular channel c. The basic idea is to couple the appropriate angular momenta in some convenient manner so that the symbol c may be used to describe a definite quantum state of the compound system[18,52]. Thus, in the "j-j coupling" c channel representation, the channel index $c \equiv [\alpha_1\alpha_2\{(ls)jI\}JM_J]$ incorporates the quantum states α_1 and α_2 of the corresponding particles and the spin s and the relative orbital angular momentum l of the projectile are coupled vectorially to give total angular momentum j. The coupling of this quantity with the total angular momentum

(spin) of the target i.e. I , yields total angular momentum J and its projection along the z-axis, M_J . If the channel spin S is invoked, the j-j representation may be replaced by $c \equiv [\alpha\{(Is)Sl\}JM_J]$. Moreover, for the sake of simplicity only elastic and inelastic channels will be dealt with; although rearrangement channels can be accommodated in the overall formulation.

The Schrödinger equation for the reaction (2.2.1) can be written in the form:

$$(H-E)\psi = (H_0+H_1-E)\psi = 0 \ , \qquad (2.2.2)$$

where the wave function ψ spans the configuration space of the complete system and the total Hamiltonian H is such that the interaction H_1 can be separated from the kinetic Hamiltonian H_0 . The crucial mathematical problem in the treatment of all nuclear reactions involving one or more open channels is that the momentum operator and functions of it such as H or $(H-E)^{-1}$ are no longer Hermitian on $(0, a_c)$. Since the Hermiticity of H is related to the validity of certain mathematical operations such as the commuting of differentiation and summation, H can not commute with the summation over a complete set of states defined in the internal region[48,51,53] .It has been shown that the difficulty arises from the non-vanishing of certain surface elements and may be circumvented by making H "realizable"[48,51,135] . This is done by adding the quantity $L(b)\psi$ to both sides of eq. (2.2.2),

$$(H+L(b)-E)\psi = L(b)\psi \ , \qquad (2.2.3)$$

where the quantity

$$L(b) = \sum_c \frac{\hbar^2}{2\mu_c} |\phi_c)\delta(r_c-a_c)\left\{\frac{d}{dr_c} - \frac{(b_c-1)}{a_c}\right\}(\phi_c| \ , \qquad (2.2.4)$$

defines the Bloch L-operator, μ_c is the reduced mass of the system in

channel c and b stands for the set of boundary condition parameters b_c which in general can be any prescribed real or complex number. The (channel) surface functions $|\phi_c)$ are functions of the intrinsic and angular variables of the system and do not depend upon the radial distance r_c. Different channel surface functions are orthogonal to one another and can be normalized, i.e.

$$(\phi_c|\phi_d) = \delta_{cd} , \tag{2.2.5}$$

where the rounded brackets denote integration over all the coordinates except r_c. The explicit form of these functions will be given later.

By using the operator inversion technique, equation (2.2.3) can be solved formally i.e.

$$\psi = [H+L(b)-E]^{-1}L(b)\psi = GL(b)\psi , \tag{2.2.6}$$

where G represents the Green function corresponding to the total Hamiltonian. Consider another set, say $\tilde{b}$, of certain parameters $\tilde{b}_c$ and define the quantity

$$\Delta L = L(\tilde{b}) - L(b) , \tag{2.2.7}$$

with the assertion that the set of states associated with the operator $L(\tilde{b})$ are the eigenstates of an arbitrary Hamiltonian $\tilde{H}$ which differs from the total Hamiltonian by the quantity

$$\Delta H = H - \tilde{H} . \tag{2.2.8}$$

Let the complete set of states $|p\rangle$ be such that

$$(\tilde{H}-E_p)|p\rangle = 0 , \tag{2.2.9}$$

with

$$L(\tilde{b})|p\rangle = 0 , \tag{2.2.10}$$

and

$$\tilde{G} = [\tilde{H}+L(\tilde{b})-E]^{-1} . \tag{2.2.11}$$

Defining the quantity

$$H = \Delta H - \Delta L \ , \tag{2.2.12}$$

one can write [Appendix (2.2A1)]

$$G = \tilde{G} - \tilde{G}HG \ , \tag{2.2.13}$$

which implies that the total Green function may be written in the form

$$G = (1+\tilde{G}H)^{-1}\tilde{G} \ . \tag{2.2.14}$$

This prescription enables one to project eq. (2.2.6) into a form suitable for further development. Since the eigenstates $|p\rangle$ belong to a complete orthonormal basis, viz.

$$\sum_{p=1}^{\infty} |p\rangle\langle p| = 1 \ , \tag{2.2.15}$$

one can write(*)

$$\tilde{G} = \sum_{p} \frac{|p\rangle\langle p|}{E_p - E} \ , \tag{2.2.16}$$

and

$$G = \left[1 + \sum_{p} \frac{|p\rangle\langle p|}{E_p - E} H\right]^{-1} \left[\sum_{q} \frac{|q\rangle\langle q|}{E_q - E}\right] \ , \tag{2.2.17}$$

where use has been made of eqs. (2.2.9)-(2.2.11) and (2.2.14). The last equation can be simplified by using the definition of the Green function in eq. (2.2.6) and making repeated use of eq. (2.2.15), viz.

$$G = \sum_{p,q} |p\rangle \left(A^{-1}\right)_{pq} \langle q| \ , \tag{2.2.18}$$

where

$$\left(A^{-1}\right)_{pq} = \langle p|G|q\rangle \ . \tag{2.2.19}$$

Finally, if

(*) In principle, the completeness relation should be written as $\sum_{p} |p\rangle\langle \hat{p}| = 1$ where $|\hat{p}\rangle = [K|p\rangle]^*$ i.e. the complex conjugate of the time reversed state; K being the usual time reversal operator[48]. However, in order to simplify notations, the symbol $\hat{}$ will not be made explicit throughout the present context.

$$B_{pq} = E_p \delta_{pq} + \langle p|H|q\rangle \ , \qquad (2.2.20')$$

$$E_{pq} = E\delta_{pq} \ , \qquad (2.2.20'')$$

it can be shown [Appendix (2.2A2)] that

$$A = (B-E) \ . \qquad (2.2.21)$$

Up till now the procedure for solving the Schrödinger equation for the reaction (2.2.1) has been kept quite formal. The Lane and Robson[48] version of the Wigner-Eisenbud R-matrix theory may, however, be crystallized by incorporating the following specifications:

i) The basis states are the eigenstates of the total Hamiltonian (i.e. $\Delta H = 0$).

ii) These states are orthogonal in the internal region.

iii) The corresponding eigenvalues (i.e. the quantities E_p etc.) are real.

iv) The basis states satisfy arbitrarily chosen real and energy independent boundary conditions at the surface of each channel; a suitable choice may be the value

$$\tilde{b}_c = \left[r_c \frac{d}{dr_c}\{ln\ \omega_{pc}(r_c)\}\right]_{r_c=a_c} \ , \qquad (2.2.22)$$

where $\omega_{pc}(r_c)$ is the radial function associated with $|p\rangle$.

v) The total wave function is expanded in terms of a complete set of states in the internal region; viz.

$$\psi = \sum_{p=1}^{\infty} C_p|p\rangle \ , \qquad (2.2.23)$$

where C_p are the expansion coefficients.

vi) ψ may satisfy the outgoing wave boundary conditions at different channel surfaces; i.e.

$$b_c = \left[r_c \frac{d}{dr_c}\{ln\ O_c(r_c)\}\right]_{r_c=a_c} \ , \qquad (2.2.24)$$

where the wave function $O_c(r_c)$ will be specified later.

With this prescription, it is straight-forward to solve eq. (2.2.6); in obvious notation

$$|\psi\rangle = GL(b)|\psi\rangle$$

$$= \sum_{p,q} |p\rangle (A^{-1})_{pq} \langle q|L(b)|\psi\rangle \,, \qquad (2.2.25)$$

and for $r_{c''} = a_{c''}$,

$$\langle q|L(b)|\psi\rangle = \sum_{c''} \langle q|\phi_{c''}\rangle \frac{\hbar^2 a_{c''}}{2\mu_{c''}} \left[\left\{\frac{d}{dr} r - b_{c''}\right\}(\phi_{c''}|\psi\rangle)\right] \,, \qquad (2.2.26)$$

where the subscript representing the channel dependence of the radial coordinates has been dropped for simplicity. Projection on to the surface functions gives the set of equations

$$(\phi_{c'}|\psi\rangle = \sum_{c''} R_{c'c''}\left[\left\{\frac{d}{dr} r - b_{c''}\right\}(\phi_{c''}|\psi\rangle)\right]_{r=a_{c''}} \,, \qquad (2.2.27)$$

where the matrix elements

$$R_{c'c''} = \sum_{p,q} \left(\frac{\hbar^2 a_{c'}}{2\mu_{c'}}\right)^{\frac{1}{2}} (\phi_{c'}|p\rangle (A^{-1})_{pq} \langle q|\phi_{c''}) \left(\frac{\hbar^2 a_{c''}}{2\mu_{c''}}\right)^{\frac{1}{2}} \,, \qquad (2.2.28)$$

constitute an R-matrix which connects the physical wave function and its derivative at the surface of the internal region. A further insight into the structure of the R-matrix may be obtained by analysing the so-called level-matrix A . Since

$$\langle p|\Delta L|q\rangle = \sum_c \gamma_{pc}\gamma_{qc}(b_c - \tilde{b}_c) \,, \qquad (2.2.29)$$

where the reduced width amplitudes are defined as

$$\gamma_{\nu c} = \left(\frac{\hbar^2 a_c}{2\mu_c}\right)^{\frac{1}{2}} (\phi_c|\nu\rangle_{r=a_c} \,, \qquad (2.2.30)$$

one can write with the help of eq. (2.2.21)

$$A_{pq} = (E_p - E)\delta_{pq} + \sum_c \gamma_{pc}\gamma_{qc}(\tilde{b}_c - b_c) \,. \qquad (2.2.31)$$

The channel-matrix character of A may be exhibited by starting from eq. (2.2.19), viz.

$$(A^{-1})_{pq} = \langle p | [1+\tilde{G}H]^{-1} \left[\sum_{p'} \frac{|p'\rangle\langle p'|}{E_{p'}-E} \right] |q\rangle$$

$$= \langle p | [1 + \tilde{G}\Delta L + \tilde{G}\Delta L\tilde{G}\Delta L + \ldots] |q\rangle / (E_q - E) \quad , \qquad (2.2.32)$$

where use has been made of the form of the Green function given by eq. (2.2.17) together with the assumption (i) i.e. $H = -\Delta L$. Substitution into eq. (2.2.28) gives

$$R_{c'c''} = R_{c'c''}(\tilde{b}) + \sum_{\bar{c}\bar{c}'} R_{c'\bar{c}'}(\tilde{b}) L_{\bar{c}'\bar{c}} R_{\bar{c}c''}(\tilde{b})$$

$$+ \sum_{\bar{c}\bar{c}'\bar{c}''\bar{c}'''} R_{c'\bar{c}'''}(\tilde{b}) L_{\bar{c}'''\bar{c}''} R_{\bar{c}''\bar{c}'}(\tilde{b}) L_{\bar{c}'\bar{c}} R_{\bar{c}c''}(\tilde{b}) + \ldots$$

$$= \sum_{\bar{c}} [1 - R(\tilde{b})L]^{-1}_{c'\bar{c}} R_{\bar{c}c''}(\tilde{b})$$

$$= \sum_{\bar{c}} R_{c'\bar{c}}(\tilde{b}) [1 - LR(\tilde{b})]^{-1}_{\bar{c}c''} \quad , \qquad (2.2.33)$$

where

$$R_{c'c''}(\tilde{b}) = \sum_{p} \gamma_{pc'} \gamma_{pc''} / (E_p - E) \quad , \qquad (2.2.34)$$

and

$$L_{c'c''} = (b_{c'} - \tilde{b}_{c'}) \delta_{c'c''} \quad . \qquad (2.2.35)$$

An instructive form of $R(\tilde{b})$ is obtained by rearranging the terms in eq. (2.2.33), viz.

$$R(\tilde{b}) = R(1+LR)^{-1} \quad , \qquad (2.2.36)$$

which reduces to a more convenient form if the total wave function satisfies zero slope boundary conditions in each channel i.e. for all c , $b_c \equiv 0$;

$$R(\tilde{b}) = R_0 (1 + L_0 R_0)^{-1} \quad , \qquad (2.2.37)$$

where the subscripts have obvious significance.

For practical applications, once a particular form of the R-matrix has been selected(*), it is straightforward to calculate the scattering matrix and hence the reaction cross sections by employing the asymptotic form of the total wave function. For $r \geq a_c$, the asymptotic form of ψ for incoming waves in the incident channel (c) may be written as

$$\psi = \sum_{c'} \left[I_{c'} \delta_{cc'} - S_{cc'} O_{c'} \right] , \qquad (2.2.38)$$

where $S_{cc'}$ is the usual scattering-matrix element and I_c (O_c) describe unit flux incoming (outgoing) particle waves and the target (residual) nucleus; viz.

$$I_c = \frac{I_c | \phi_c)}{V_c^{\frac{1}{2}} r_c} = O_c^* \qquad (2.2.39)$$

where V_c is the relative velocity of the pair in channel c and I_c and O_c are the two linearly independent solutions of the radial equation[18].

The surface functions are of the following form(**)

$$| \phi_c) = \Phi_\alpha(\zeta) \sum_{m_l m_S} C(lSJ | m_l m_S M_J) i^l Y_l^{m_l}(\theta, \phi) \chi_S^{m_S}(\sigma) , \qquad (2.2.40)$$

(*) It may be worthwhile spending a few words about the nomenclature of the different forms of R-matrices introduced so far. Form (2.2.28) with prescription (2.2.27) is the most general form of the R-matrix involving arbitrary boundary condition sets b and $\tilde{b}$ and has been designated by Lane and Robson[50] as the "Wigner-Eisenbud calculable R-matrix". It may be alternatively referred to as the "level-form of the R-matrix". On the other hand, form (2.2.33) can be convenient for those cases in which very few channels but many levels are involved. This form will be referred to as the "channel-form of the R-matrix". The form in eq. (2.2.34) exhibits a special case which could be obtained by putting $b = \tilde{b}$ either in eq. (2.2.33) or in eq. (2.2.31). The latter yields a diagonalized A-matrix which - when substituted in eq. (2.2.27) with $b_c = \tilde{b}_c$ - gives the so-called Lane and Thomas[18] version of the Wigner-Eisenbud R-matrix theory. Finally, the forms in eqs. (2.2.36) and (2.2.37) are some special cases which will be useful in the forthcoming developments.

(**) Notice that the present form differs from that of Lane and Thomas[18] in the coupling scheme and the lack of a factor r_c^{-1}.

where $\Phi_\alpha(\zeta)$ is the wave function of the internal coordinates ζ, $\chi_S^{m_S}(\sigma)$ is the (channel) spin function, $C(|)$ represents a Clebsch-Gordan coefficient and the remaining symbols have their usual significance. Consequently, for channels of a fixed partition of particles between the target and the projectile, one can write

$$\psi = \sum_c r_c^{-1} u_c(r_c) |\phi_c) \ , \tag{2.2.41}$$

$$|p\rangle = r_c^{-1} \omega_{pc}(r_c) |\phi_c) \ , \tag{2.2.42}$$

and

$$(\phi_c|p\rangle = r_c^{-1} \omega_{pc}(r_c) \ . \tag{2.2.43}$$

The above results enable one to show (Appendix (2.2A3)] that for outgoing wave boundary conditions, say $b_c^0 \in \{b^0\}$, the scattering-matrix can be written in the form(*)

$$S_{cc'} = i\hbar^{-1}\left[\langle O_{c'}|L(b^0)|I_c\rangle + \langle O_{c'}|L^*(b^0) - L(b^0)|\psi\rangle\right] \ , \tag{2.2.44}$$

or

$$S_{cc'} = \frac{I_c(a_c)}{O_c(a_c)} \delta_{cc'} + i \frac{(2k_c a_c)^{\frac{1}{2}}}{O_c(a_c)} R_{cc'} \frac{(2k_{c'} a_{c'})^{\frac{1}{2}}}{O_{c'}(a_{c'})} \ , \tag{2.2.45}$$

where use has been made of equation (2.2.25) and $k_c = \rho_c/a_c = \mu_c V_c/\hbar$. Thus, once the S-matrix has been evaluated, the elastic- or inelastic-reaction cross section can be obtained by using the appropriate relations.

The R-matrix theory discussed so far is quite general and the arbitrariness in the choice of boundary condition parameters $\tilde{b}_c$ does not

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(*) Alternatively, the substitution of eq. (2.2.38) in both sides of eq. (2.2.27) gives the following expression in standard notation[18],

$$S = \rho^{\frac{1}{2}}[O(1-RL^0)]^{-1}[(1-RL^{0*})I]\rho^{-\frac{1}{2}} \ , \tag{2.2.46}$$

where ρ, O and I are the diagonal matrices defined earlier and L^0 is given by eq. (2.2.35) with $b_{c'} = b_{c'}^0$.

play a very conspicuous role in the sense that the evaluation of any measurable quantity with a particular set of $\tilde{b}_c$ can be reporduced exactly for any other set of $\tilde{b}_c$ values[137]. This is due to the dependence of the level parameters γ_{pc} and E_p on the choice of $\tilde{b}_c$ and a_c.

In practical applications, the general R-matrix theory necessarily requires a truncation of the infinite dimensional spaces spanned by the basis states and channels. This introduces three approximations into the theory: (i) the sum in eq. (2.2.23) is not exhausted completely; (ii) a non-rigorous treatment of the completeness relation (2.2.15); (iii) the neglect of typical two-, three- and many-body channels. Notice that the treatment of the last approximation can give rise to an exceedingly complicated theory(*). These considerations imply that unless the effect of all the neglected terms is retained, which is quite impracticable in actual calculations, the present form of the R-matrix theory may not be quite suitable to predict the converged results for a definite reaction. However, in view of the flexibility in the choice of channel radii, one can find certain boundary condition dependent level parameters which can fit the experimental results. This becomes laborious[138] and even impossible when many channels and/or many levels are involved. Finally, the level parameters do not have any particular physical significance so that one can not learn much about the internal dynamics of the nuclei involved.

2.3 Standard R-matrix method

As emphasized in the previous section, the main disadvantage of employing the R-matrix theory has been the inadequacy of the theory to predict reasonable estimates of the reaction cross section. Moreover, the

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(*) This problem has been tackled recently in a systematic way by D. Robson[52].

insufficient physical significance of the level parameters in relation to the proper nuclear dynamics within the internal region introduces additional arbitrariness in the theory. However, developments in the theory of nuclear structure (i.e. the shell- and collective-models) have made it possible to predict fairly precisely many characteristic features of the low-lying states of nuclei[139]. Consequently, in order to give a concrete physical significance to the level parameters, it is desirable to obtain the structure of the compound nucleus involved in the R-matrix theory through some properly studied nuclear model.

The problem of incorporating a nuclear model in order to describe the reaction cross sections has been tackled in several other forms. The conventional shell model[43,44] with harmonic oscillator basis functions, for example, is not quite sufficient since the cross sections can not be predicted satisfactorily due to the incorrect asymptotic behaviour of the corresponding wave functions and the neglect of physical boundary conditions. In other words, although the model has been very successful in describing the "volume" characteristics (e.g. excitation energies, beta decay and electromagnetic transition rates) of nuclei; it is unable to describe satisfactorily the nuclear "surface" characteristics such as alpha decay, direct reactions and the decay of compound states in the external region. Among other alternatives are the theories which eliminate the concept of boundary conditions in favour of variations in the nuclear Hamiltonian[77-79,130-134]. Based upon the coupled-equations theory of Feshbach, these theories may be inadequate in some cases due to the difficulties in constructing the appropriate projection operators, the occurrence of continuum states and the problems in dealing with realistic effective interactions. Finally, although a straightforward coupled-channels formulation may be utilized to obtain the exact solutions of the simple reaction problems, it may not be feasible to deal with complicated reactions involving more realistic physical models.

Haglund and Robson[47] have propounded the idea of modifying the conventional R-matrix theory by using a set of discrete compound nucleus states which can be obtained from the well known shell model techniques. In fact the standard R-matrix (SRM) method can be derived from the general formalism developed in the previous section by modifying the condition (i) [i.e. $\Delta H = 0$] to incorporate a definite value of the residual interaction, which gives rise to the coupling among different channels when extrapolated within the internal region. In this way a set of basis functions is generated through a simple form of the model Hamiltonian (which is assumed to be diagonal in the channel space) and the matrix involving the residual interaction is diagonalized to yield the resultant R-matrix. The latter can be treated in the usual way to predict the cross sections and the related measurable quantities.

Thus, in practice, the SRM method suggests an alternative route for solving the coupled-channels problem. This method will be elaborated in the following paragraphs by making use of the Bloch operator formalism developed in the previous section.

Consider the total Hamiltonian of the system in the form

$$H = T + H_t + H_d + H_c = H_0 + H_1 \ , \qquad (2.3.1)$$

where T is the (relative) kinetic energy operator and H_t is the target Hamiltonian giving rise to different target states of energy ε_c ; viz.

$$(H_t - \varepsilon_c)|\phi_c) = 0 \ . \qquad (2.3.2)$$

The quantity H_d (H_c) represents that part of the interaction Hamiltonian which is diagonal (non-diagonal) in the channel space. Thus the Schrödinger equation (2.2.2) with Hamiltonian (2.3.1) and the expansion (2.2.41) of the total scattering wave function ψ give the set of coupled equations

$$[T + (\phi_c|H_d|\phi_c) + \varepsilon_c - E]u_c(r) = -\sum_{c'} (\phi_c|H_1|\phi_{c'})u_{c'}(r) \qquad (2.3.3)$$

where H_1 stands for the coupling Hamiltonian H_c .

The SRM method of solving the above set of equations is based on the introduction of the so-called "channel R-matrix states" which are the eigenstates of the model Hamiltonian H_0 $(= T + H_t + H_d)$ in the internal region;

$$\left(H_0 - E_p^{(0)}\right) |p, c\rangle = 0 \ , \quad r_c \leq a_c \ . \tag{2.3.4}$$

These eigenstates satisfy energy-independent and homogeneous boundary conditions at the surface

$$L(\tilde{b}) |p, c\rangle = 0 \ , \tag{2.3.5}$$

and resemble in all respects the eigenstates $|p\rangle$ defined in the previous section except that the channel index c has been made explicit for the sake of clarification. The associated (uncoupled) reduced width amplitudes may be defined by making use of eq. (2.2.43) in the form

$$\zeta_{pc} = \left(\hbar^2/2\mu_c a_c\right)^{\frac{1}{2}} \omega_{pc}(a_c) \ , \tag{2.3.6}$$

and the associated Green function is defined as

$$G_0(\tilde{b}) = \left(H_0 + L(\tilde{b}) - E\right)^{-1} \ . \tag{2.3.7}$$

Defining the "coupled R-matrix states" $|\psi_\lambda\rangle$ as solutions of the equation(*)

$$\left(H + L(\tilde{b}) - E_\lambda\right) |\psi_\lambda\rangle = L(\tilde{b}) |\psi_\lambda\rangle \ , \quad r_c \leq a_c \ , \tag{2.3.8}$$

satisfying the energy-independent boundary conditions

$$L(\tilde{b}) |\psi_\lambda\rangle = 0 \ , \tag{2.3.9}$$

at the surface, one may write the corresponding Green function as

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(*) Notice that in the R-matrix theory the eigenstates of H coincide with those of $\tilde{H}$ due to the vanishing of the residual interaction ΔH in the internal region. As the coupling interaction becomes finite $(\Delta H \neq 0)$, it is necessary to distinguish between the corresponding eigenstates (i.e. $|p, c\rangle$ and $|\psi_\lambda\rangle$ in the present case) within the internal region although they satisfy the same boundary conditions at the surface.

$$G(\tilde{b}) = \left(H+L(\tilde{b})-E\right)^{-1} = \sum_{\lambda} \frac{|\psi_\lambda\rangle\langle\psi_\lambda|}{(E_\lambda-E)} , \qquad (2.3.10)$$

where use has been made of the assertion that the eigenstates $|\psi_\lambda\rangle$ form a complete orthonormal set. This Green function is connected to the total Green function G [*cf.* eqs. (2.2.6) and (2.2.14)] and $G_0(\tilde{b})$ through the relations

$$G(\tilde{b}) = [1-G(\tilde{b})\Delta L]G , \qquad (2.3.11)$$

and

$$G(\tilde{b}) = \left[1+G_0(\tilde{b})H_1\right]^{-1}G_0(\tilde{b}) . \qquad (2.3.12)$$

In deriving the last relation it is understood that the eigenstates $|\psi_\lambda\rangle$ and $|p, c\rangle$ satisfy the same boundary conditions so that relation (2.2.14) can be utilized by substituting $\Delta L = 0$ and $\Delta H = H_1$.

The channel-form of the R-matrix can now be obtained by employing eq. (2.3.10), viz.

$$R_{c'c''} = \left(\frac{\hbar^2}{2\mu_{c'}a_{c'}^3}\right)^{\frac{1}{2}} \langle \delta(r_{c'}-a_{c'})(\phi_{c'}|G(\tilde{b})|\phi_{c''})\delta(r_{c''}-a_{c''})\rangle \left(\frac{\hbar^2}{2\mu_{c''}a_{c''}^3}\right)^{\frac{1}{2}}$$

$$= \sum_{\lambda} \gamma_{\lambda c'}\gamma_{\lambda c''}/(E_\lambda-E) , \qquad (2.3.13)$$

with the "coupled" reduced width amplitudes defined as

$$\gamma_{\lambda c} = \left(\frac{\hbar^2}{2\mu_c a_c}\right)^{\frac{1}{2}} \psi_{\lambda c}(a_c) . \qquad (2.3.14)$$

Notice that the form (2.3.13) of the R-matrix could be derived from relation (2.2.33) by taking $b = \tilde{b}$ and defining the corresponding reduced width amplitudes according to eq. (2.3.14) where use has been made of the expansion

$$|\psi_\lambda\rangle = \sum_{c} r_c^{-1}\psi_{\lambda c}(r_c)|\phi_c) . \qquad (2.3.15)$$

Since the basis states $|p, c\rangle$ generate a complete orthonormal set for

$r_c \leq a_c$, the coupled R-matrix states $|\psi_\lambda\rangle$ may be expanded in terms of them; viz.

$$|\psi_\lambda\rangle = \sum_p C_{\lambda p} |p, c\rangle \ . \qquad (2.3.16)$$

Substitution of the above expansion into equation (2.3.8) yields the infinite set of equations

$$\sum_{p=1}^{\infty} C_{\lambda p}\left[\left(E_p^{(0)} - E_\lambda\right)\delta_{pp'}\delta_{cc'} + \langle p', c'|H_1|p, c\rangle\right]$$

$$+ \langle p', c'|L(\tilde{b})|\psi_\lambda\rangle = 0 \ . \qquad (2.3.17)$$

In practice, however, only a finite number of states, say ν , is taken into account so that one can write

$$\sum_{p=1}^{\nu} C_{\lambda p}\left[\left(E_p^{(0)} - E_\lambda\right)\delta_{pp'}\delta_{cc'} + \langle p', c'|H_1|p, c\rangle\right] = 0 \ , \qquad (2.3.18)$$

or in matrix form

$$C\left(E^{(0)} + H_1\right) = EC \ , \qquad (2.3.19)$$

where $E^{(0)}$ and E are diagonal matrices with the remaining symbols having obvious significance and noting that condition (2.3.9) is used.

With this prescription, the overall procedure for calculating the R-matrix [eq. (2.3.13)] with the SRM method may be summarized as follows:

(i) Determine the various states $|p, c\rangle$ and the corresponding energy levels E_p in each channel by solving the characteristic equation (2.3.4).

(ii) Establish the matrix elements of the residual interaction with the help of previously determined states $|p, c\rangle$ and the given form of H_1 .

(iii) Diagonalize the set of equations (2.3.18) to obtain the eigenvalues E_λ and the expansion coefficients $C_{\lambda p}$

which in turn give the coupled R-matrix states $|\psi_\lambda\rangle$.

(iv) Obtain the coupled reduced width amplitudes either through relation (2.3.14) or directly, i.e.

$$\gamma_{\lambda c} = \sum_p C_{\lambda p}\zeta_{pc} \tag{2.3.20}$$

and formulate the R-matrix through eq. (2.3.13).

Of course, once the R-matrix is obtained, it is straightforward to determine the scattering matrix and hence the cross sections, either by employing the method described in the last section or solving the set of coupled equations:

$$[\tilde{I}_c\delta_{cc'}-S_{cc'}\tilde{O}_{c'}]V_{c'}^{-\frac{1}{2}} = \sum_{c''} R_{c'c''}[(r\tilde{I}_{c''})'\delta_{cc''} - S_{cc''}(r\tilde{O}_{c''})'-b_{c''}\{\tilde{I}_{c''}\delta_{cc''}-S_{cc''}\tilde{O}_{c''}\}]_{r=a_{c''}} V_{c''}^{-\frac{1}{2}} , \tag{2.3.21}$$

which is obtained by substituting equations (2.2.4), (2.2.38) and (2.2.41) into the relation

$$(\phi_{c'}|\psi\rangle = (\phi_{c'}|G(\tilde{b})L(b)|\psi\rangle \tag{2.3.22}$$

and making use of the definitions (2.3.10) and (2.3.13). Notice that $\tilde{I}_c \equiv I_c r^{-1}$, V_c is the velocity in channel c and the choice of boundary condition parameters b_c is left arbitrary.

In order to test the validity of the SRM method, Haglund and Robson applied it to an exactly soluble problem[47,140] by considering a set of equations of the type (2.3.3) in which two square-well potentials are coupled through a square-well. Apart from some computational inaccuracies in the very low-energy region, the agreement between the "predicted" cross section with six levels per channel in the SRM calculations and "exact" cross sections was found to be satisfactory over a reasonably wide range of energies.

Buttle[63] employed a more sophisticated model (i.e. a real Woods-Saxon potential plus a spin-orbit term of the Thomas form for the diagonal potential and a rotational model[86] for the coupling potential) for studying the inelastic- and elastic-scattering reactions of nucleons incident on a ^{12}C target. His SRM calculations give good qualitative agreement with the corresponding coupled-channels results. He has found, however, that a consistent error of the SRM method is to overestimate the elastic forward peak when three levels per channel are used.

These initial tests and some later studies[97,98] have suggested that although the SRM method can be regarded as an outstanding means of calculating the cross sections in the resonant as well as the non-resonant regions from a given nuclear model, it sometimes requires quite a large number of basis states.

2.4 Generalized *R*-matrix method

It was shown in the last section that, given a model Hamiltonian, one can generate the reaction cross section in a calculable way by employing the SRM method. However, since in the practical application of this method one has to use a truncated series, some arbitrariness is introduced in the overall formulation which tends to give problems when a desirable accuracy is required over a wide range of energy. A critical analysis of the method shows that there is some flexibility in the choice of the boundary condition parameters, the size of the internal region and the basis states generated through the nuclear model. Thus, Tobocman and Nagarajan[58] have "generalized" the SRM method by "extending" the ideas therein to accommodate basis states which satisfy real but "inhomogeneous" boundary conditions and are "non-orthogonal" over the internal region. Later on, the method was further

developed by Lane and Robson[50,51,141] within the framework of the "calculable theories of reactions based on the shell model".

Although the formulation of the generalized R-matrix (GRM) method can be established by extending the results obtained in sections 2.2 and 2.3; in what follows the GRM method will be discussed in full for the sake of completeness. Thus, starting from the Schrödinger equation

$$\left(H+L(b)-E\right)\psi_G = L(b)\psi_G \qquad (2.4.1)$$

for the system discussed in the preceding sections, the ultimate goal is to determine the wave function ψ_G satisfying the appropriate boundary conditions at the surface of the internal region. According to the GRM method, the Hamiltonian of the system in the internal region can be replaced by a model Hamiltonian H_M which is composed of a core Hamiltonian H_c, a single-particle Hamiltonian H_s and the residual interaction H_R, i.e.

$$H_M \equiv H = H_c + H_s + H_R \,, \qquad (2.4.2)$$

and therein the model wave function ψ_M is assumed to be expressible in terms of a finite set of basis states ψ_λ, viz.

$$\psi_M \equiv \psi_G = \sum_{\lambda=1}^{N} C_\lambda \psi_\lambda \qquad (2.4.3)$$

with the amplitudes C_λ corresponding to the appropriate expansion coefficients. Although the selection of the basis states ψ_λ is left arbitrary; they should, in principle, be chosen such that the model wave function ψ_M, when represented by a minimum number of basis functions within the internal region and at all $r_c = a_c$, gives rise to a sufficiently accurate estimate of the reaction cross section. In an attempt to achieve this, the GRM method takes into account the following considerations regarding the behaviour of basis states:

(i) NON-ORTHOGONALITY: On account of the non-orthogonality of the basis

functions, one has to introduce a more general completeness relation than the one given by eq. (2.2.15):

$$1 = \sum_{\lambda,\nu=1}^{\infty} |\psi_\lambda\rangle N^{\infty}_{\lambda\nu} \langle\psi_\nu| \tag{2.4.4}$$

where $N^{\infty}_{\lambda\nu}$ is the element of the non-orthogonality matrix. Following Lane and Robson[50] this exact unit operator can be written as

$$1 = \sum_{\lambda,\nu=1}^{N} |\psi_\lambda\rangle N_{\lambda\nu} \langle\psi_\nu| + \sum_{i,j=N+1}^{\infty} |\psi_i\rangle X_{ij} \langle\psi_j| \tag{2.4.5}$$

where the first term corresponds to the so-called "nearby" space, the second term to the remainder and the matrices N and X are left unspecified for the moment. For practical purposes one has to use the truncated series of eq. (2.4.3) and the exact unit operator in eq. (2.4.5) is approximated by

$$1 = \sum_{\lambda,\nu=1}^{N} |\psi_\lambda\rangle N_{\lambda\nu} \langle\psi_\nu| \quad , \quad r_c = a_c \ . \tag{2.4.6}$$

The matrix N satisfies the equation

$$\mathsf{ONO} = \mathsf{O} \ , \tag{2.4.7}$$

which leads to the solution

$$\mathsf{N} = \mathsf{O}^{-1} \ , \tag{2.4.8}$$

where the elements of the "overlap" matrix are given by

$$O_{\lambda\mu} = \langle\psi_\lambda|\psi_\mu\rangle \tag{2.4.9}$$

with the assumption that the range of the radial integral extends from 0 to a_c and the inverse of O exists.

(ii) CHOICE OF POTENTIAL MODEL: The arbitrary set of basis states

$$\psi_\lambda \equiv r_c^{-1} \omega_{\lambda c}(r_c) |\phi_c) \tag{2.4.10}$$

is to be fixed in terms of the corresponding channel states by a suitable choice of the radial function $\omega_{\lambda c}(r_c)$. This may be done in terms of the

eigenstates of the Hamiltonian

$$H_0 = H_M - H_R = H_c + H_s \tag{2.4.11}$$

with the single-particle Hamiltonian defined as

$$H_s = T_s + V_s(r_c) \ , \tag{2.4.12}$$

where T_s is the single-particle kinetic energy operator and $V_s(r_c)$ is a central potential. Actually, the selection of $\omega_{\lambda c}(r_c)$ and hence of ψ_λ is based on the specific nature of this potential. When combined with H_c and H_R , $V_s(r_c)$ should be such that the overall structure of the intermediate system can be expressed in terms of a reliable nuclear model e.g. the shell model. In practice, however, one may choose either a potential with infinite well depth e.g. a harmonic oscillator (h.o.) potential or some realistic potential of finite well depth e.g. the Woods-Saxon potential.

In view of the simple analytic nature of the corresponding wave functions and the extreme convenience in their use, most of the GRM method calculations employ the h.o. potential[67,75,121]; although the Woods-Saxon or any other finite depth potential can be handled equally well as far as the computation is concerned. The difference lies, however, in the characteristics of the corresponding set of basis states. As is well known, the h.o. potential gives rise to a denumerably infinite set of discrete energy levels and hence a complete set of discrete wave functions, say $\omega_{\lambda c}(r_c)$, from which the desired model wave functions can be generated in the usual way[44,142]. The h.o. wave functions, however, die out at infinity due to the absence of any continuum and the higher orbitals no longer remain even approximately orthogonal within the specific internal region. Whereas the former characteristic inhibits the use of the h.o. basis states in theories involving no internal region [e.g. the dynamical

theories of class (ii) in Section 2.1], the latter does not give any problem due to the general non-orthogonal behaviour of the GRM method basis states established in the previous paragraphs.

On the other hand, in addition to a finite set of discrete wave functions, the finite well potential introduces an infinite set of continuous wave functions. For practical purposes, these wave functions are to be "discretized" by an appropriate choice of boundary conditions at or near the channel radii[58,189]. Consequently, one can construct a complete set of basis states incorporating these "discretized" eigenfunctions so that the usual methods of finite matrix inversion and diagonalization can be applied without any formal problem(*).

Finally, in both cases for simplicity one usually ignores the complications arising from the appearance of spurious states due to the centre of mass motion and the effect of rearrangement and three- or many-body channels.

(iii) INHOMOGENEOUS BOUNDARY CONDITIONS: Whatever may be the nature of the potential model, the basis states are required to satisfy certain boundary conditions at the various channel surfaces of the internal region. More symbolically, the eigenstates of the Hamiltonian H_0 i.e.

$$\left(H_0 - E_\lambda^{(0)}\right)|\psi_\lambda\rangle = 0 \qquad (2.4.13)$$

should be such that

$$L(\tilde{b})|\psi_\lambda\rangle = 0 \ , \qquad (2.4.14)$$

where, however, the typical nature of the set $\tilde{b}$ incorporating the energy-independent parameters $\tilde{b}_c$ is to be specified in a more general sense. In

(*) There may be difficulties arising from the fact that the complete set so formed will have configurations involving three or more particles in positive energy orbitals and the corresponding wave functions will oscillate at infinity. This in turn implies that the Hermiticity of the operator $[H+L(b)]$ appearing in eq. (2.4.1) may be maintained only if one is below the threshold for all three- or many-body channels.

contrast to the SRM method, the generalized form of these parameters results partly from the non-orthogonality of the basis states. To be more specific, in view of the definitions (2.2.4) and (2.4.14), the usual boundary condition parameters i.e.

$$\tilde{b}_c = \left[r_c \frac{d}{dr_c} \{ ln\ \omega_{\lambda c}(r_c) \} \right]_{r_c = a_c} \tag{2.4.15}$$

now become "λ-dependent" in each channel; viz.

$$\tilde{b}_c \rightarrow \tilde{b}_{c\lambda} \neq b_{c\lambda'} , \tag{2.4.16'}$$

and the "inhomogeneity" requires that

$$\tilde{b}_{c\lambda} \neq \tilde{b}_{c'\lambda'} \neq \tilde{b}_{c'\lambda} . \tag{2.4.16"}$$

The apparent advantage of employing inhomogeneous boundary conditions is the freedom of studying thoroughly the complicated situations resulting from the presence of two or more resonances in the same channel. Moreover, the flexibility in the choice of different $\tilde{b}_{c\lambda}$ may enable one to calculate rather better values of the cross sections in many-channels reaction problems.

From the above considerations, the Green function appearing in the formal solution of equation (2.4.1) within the internal region i.e.

$$\psi_G = GL(b)\psi_G , \tag{2.4.17}$$

can be written as

$$\begin{aligned} G &= \sum_{\lambda\nu\lambda'\nu'} |\psi_\lambda\rangle N_{\lambda\nu} \langle \psi_\nu | G | \psi_{\lambda'} \rangle N_{\lambda'\nu'} \langle \psi_{\nu'} | \\ &= \sum_{\lambda\lambda'} |\psi_\lambda\rangle (A^{-1})_{\lambda\lambda'} \langle \psi_{\lambda'} | , \end{aligned} \tag{2.4.18}$$

where use has been made of the relation

$$\begin{aligned} \langle \psi_\lambda | \psi_\mu \rangle &= \sum_{\nu\nu'} \langle \psi_\lambda | G | \psi_\nu \rangle N_{\nu\nu'} \langle \psi_{\nu'} | G^{-1} | \psi_\mu \rangle \\ &= N^{-1}_{\lambda\mu} , \end{aligned} \tag{2.4.19}$$

together with the definitions (2.4.6) and (2.4.8). Moreover, the matrix A

is such that

$$A_{\lambda\mu} = \langle \psi_\lambda | G^{-1} | \psi_\mu \rangle$$
$$= \left(E_\mu^{(0)} - E\right) \left[\langle \psi_\lambda | \psi_\mu \rangle\right]_0^{a_c} + \sum_c \gamma_{\lambda c} \left(\tilde{b}_{\mu c} - b_c\right) \gamma_{\mu c} + \langle \psi_\lambda | H_R | \psi_\mu \rangle \ , \tag{2.4.20}$$

which may be derived similarly to the corresponding A-matrix of the SRM method and

$$\gamma_{\nu c} = \left(\frac{\hbar^2}{2\mu_c a_c}\right)^{\frac{1}{2}} \omega_{\nu c}(a_c) \ . \tag{2.4.21}$$

Notice that for homogeneous boundary conditions the overlap integral $\langle \psi_\lambda | \psi_\mu \rangle \to \delta_{\lambda\mu}$ and eq. (2.4.20) coincides with eq. (2.2.31) for $H_R \to 0$.

This prescription enables one to write the formal solution (2.4.17) in the form

$$|\psi_G\rangle = \sum_{\lambda\lambda'} |\psi_\lambda\rangle \left(A^{-1}\right)_{\lambda\lambda'} \langle \psi_{\lambda'} | L(b) | \psi_G \rangle \ . \tag{2.4.22}$$

Projecting on to the surface functions and utilizing the expansions (2.2.38) and (2.2.41) for the GRM wave function ψ_G , one obtains a set of coupled equations identical to the set in eq. (2.3.21) for the S-matrix except that the (generalized) R-matrix is given in terms of the level-matrix of eq. (2.4.20), i.e.

$$R_{c'c''} = \sum_{\lambda\lambda'} \left(\frac{\hbar^2 a_{c'}}{2\mu_{c'}}\right)^{\frac{1}{2}} \left(\phi_{c'} | \psi_\lambda\right) \left(A^{-1}\right)_{\lambda\lambda'} \left(\psi_{\lambda'} | \phi_{c''}\right) \left(\frac{\hbar^2 a_{c''}}{2\mu_{c''}}\right)^{\frac{1}{2}} \ . \tag{2.4.23}$$

Alternatively, instead of inverting the A-matrix, one can substitute the expansion (2.4.3) directly into the Schrödinger equation (2.4.1) and get the following set of dynamical equations for the GRM method.

$$\sum_{\lambda=1}^{N} \left[\left(E_\lambda^{(0)} - E\right) \langle \psi_\mu | \psi_\lambda \rangle + \langle \psi_\mu | H_R | \psi_\lambda \rangle + \sum_c \gamma_{\mu c} \left(\tilde{b}_{\lambda c} - b_c\right) \gamma_{\lambda c}\right] C_\lambda = 0 \ , \tag{2.4.24}$$

where the parameters b_c correspond to the boundary conditions satisfied by ψ_G and the remaining symbols have their usual significance. A comparison

with eq. (2.3.17) shows that the above set of equations is an obvious generalization of the dynamical equation in the SRM method and can be solved in a similar manner.

The initial numerical test of the Tobocman and Nagarajan version of the GRM method[58] was carried out by Nagarajan *et al.*[59,143] by considering the bound state and scattering problems for a square-well potential. These calculations have qualitatively reproduced the bound state energies and the scattering phase shifts.

Since the development of precise techniques for handling the mathematical difficulties[50,51,141,152], the GRM method has found several interesting applications. Adams[144,145] has applied it to the square-well problem. Later on Purcell[121] carried out numerical calculations for various analytically soluble cases which approximate more realistic physical models; e.g. scattering by a square-well, scattering by a pair of coupled square-wells and scattering by a square-well plus a pure Coulomb potential. These tests not only revealed the usefulness of the method but also gave a familiarity with the numerical techniques necessary for the further application of the method.

Within the framework of the GRM method, Purcell[67] did the first realistic calculations for the $^{12}C(n, n)^{12}C$ reaction by employing a quadrupole deformation of a harmonic oscillator potential in the weak coupling particle-rotator model for the positive parity states of ^{13}C. Robson and Van Megen[71] have done similar calculations with a more physical choice of the residual interaction (e.g. quadrupole deformation of a Woods-Saxon potential). They have also used a simple shell-model wave function to describe the ^{12}C core and a delta function type form factor for the two-body interaction in a separate work[72]. Mori[74] has incorporated a

microscopic model for calculating the intrinsic state of ^{12}C together with more realistic (effective) two-body interactions for the interaction between the incident neutron and the core nucleons and an explicit account of the antisymmetrization effect. The common feature of these calculations is that although they reproduce the position of the resonances in the scattering cross section, the calculated widths of the resonances disagree with the observed values. In a more detailed analysis of the same problem, Philpott and George[75] used the weak vibrational model of Reynolds *et al.*[66] and found that the GRM method can predict very well the reaction cross section provided a sufficient (eight or more) number of harmonic oscillator wave functions per channel for a channel radius of about 7.0 fm is used.

Other applications of the GRM method to realistic nuclear problems are the results of Chatwin and Purcell[69] for α-α scattering and the study of $^{12}C(p, p')^{12}C$ reaction by Van Megen[146]. The former calculations give a satisfactory description of the data, but the latter, while predicting reasonable values of the resonance energies, do not give a very satisfactory description of the resonance widths. It may be worth mentioning here that the GRM method has been employed by Philpott in a series of continuum shell-model calculations[147-149] in which cases the dynamical equations of the model may be reduced to simple and elegant algebraic form.

Apart from the versatility of the GRM method in connection with studies of the bound and continuum properties of the nuclear Hamiltonian, the method is not yet free from problems. To start with, it requires a relatively large number of basis states per channel which may restrict its application to atomic and molecular problems where the number of reaction channels is large. Moreover, as the number of basis states is increased, the results ultimately diverge from the exact results. As compared with the SRM method, Westin and Adams[150,151] found in their investigations for the situations of

two closely spaced resonance levels of the same spin and parity in a channel, that the GRM method complicates numerical analysis and has the weakness that the inclusion of distant levels is impracticable. Philpott and George[75], however, insist that there is no need to invoke the effects of distant levels since the improper convergence of the method could be due to an incorrect choice of channel radii. Moreover, since boundary condition parameters b_c are explicit functions of these radii and the incident energy, they suggest a criterion for selecting the "best" set of channel radii. This criterion, however, is based on an energy dependent iterative procedure.

2.5 Corrections to the SRM method

As has been mentioned in Section 2.3, in some cases the SRM method requires a large number of basis states to achieve a satisfactory convergence. Buttle[63] has found that if the effect of the remaining basis states can also be included approximately in the usual SRM calculations, one may require a relatively smaller number of basis states.

Before describing the Buttle correction for the remaining states, it is worthwhile to have a general idea about the behaviour of *all* the basis states in any R-matrix type method. As stated earlier, the basis states in an SRM method calculation should, in principle, span an infinite dimensional Hilbert space, say H^{∞}, within the internal region so that the series expansion in eq. (2.3.16) can be satisfied exactly. Thus an "idealized" SRM method would result if one diagonalizes the set of equations (2.3.17), which may be written in more symbolic notation as

$$\mathrm{CD}^{\infty} = \mathrm{EC} \tag{2.5.1}$$

where

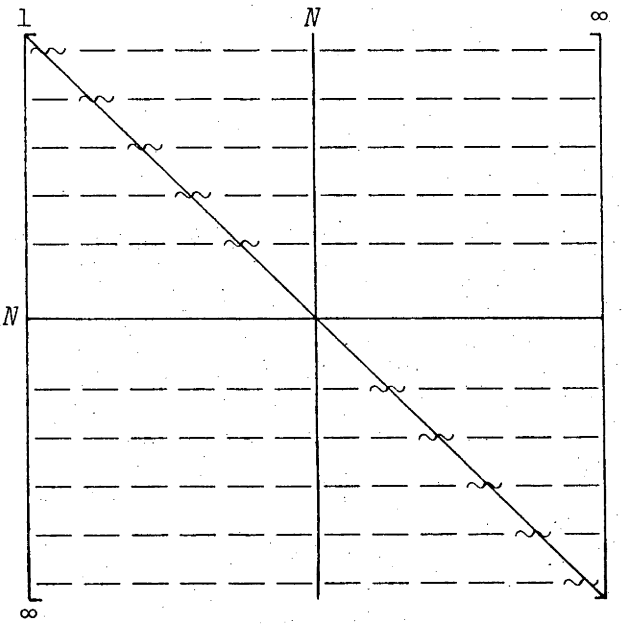
$$\mathrm{D}^{\infty} = \mathrm{H}_d^{\infty} + \mathrm{H}_n^{\infty} \tag{2.5.2}$$

and H_d^∞ and H_n^∞, respectively, represent the matrix elements of the diagonal and non-diagonal parts of the total Hamiltonian H in the space H^∞. For this case the matrix D^∞ is shown schematically in figure (2.5.1a) where the diagonal matrix elements are distinguished by light wavy lines.

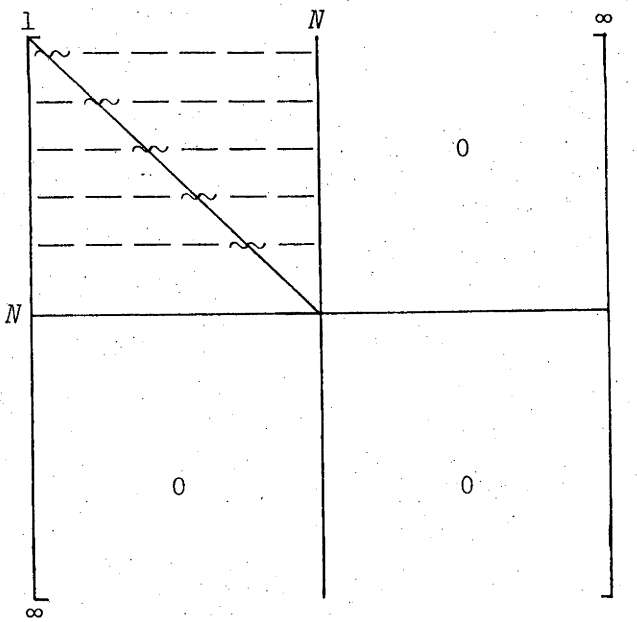
Of course, the representation in eq. (2.5.2) is far from being realistic for practical applications and one employs in the usual SRM method a severely truncated part, say H^N, of H^∞. In this case the form (2.5.1) coincides with eq. (2.3.19) since $H_d^\infty \to H_d^N$ and $H_n^\infty \to H_n^N$; as shown in figure (2.5.1b). Consequently, one can expect considerable disagreement of the SRM predictions with exactly calculated results in cases where the diagonal and non-diagonal matrix elements in the distant space H^D $(\equiv H^\infty - H^N)$ are important.

The corresponding situation for the GRM method is shown in figure (2.5.1c) where the dark wavy lines indicate that the diagonal matrix elements are modified due to the presence of the non-orthogonal states and the modification of the non-diagonal matrix elements (dark dashes) mainly results from the inhomogeneous boundary condition parameters. Whereas the SRM method uses a fixed boundary condition parameter which may lead to a poor convergence (as the number of basis states is increased) of the predicted cross sections for some energies, the GRM method which employs inhomogeneous i.e. more "random" boundary condition parameters tends to give a more reasonable convergence of the predictions over the whole energy region.

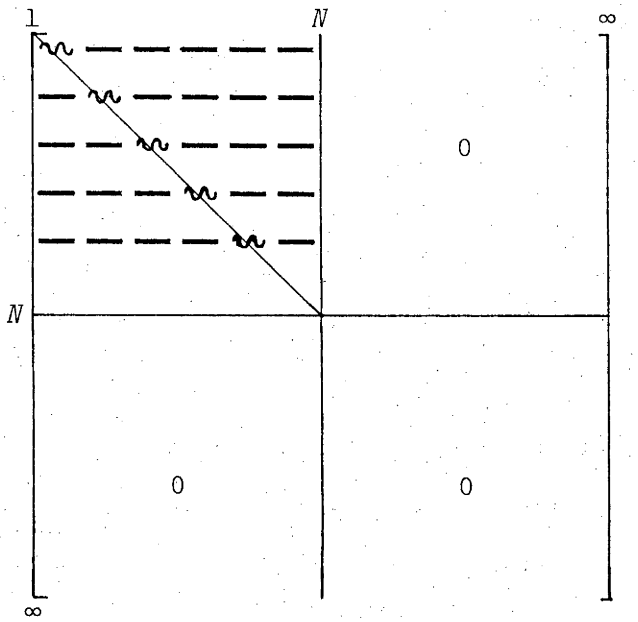
Before proceeding further it may be worth remarking that whereas the SRM method gives improved results by enlarging the truncated space, the corresponding procedure for the GRM method is not quite obvious[50] because



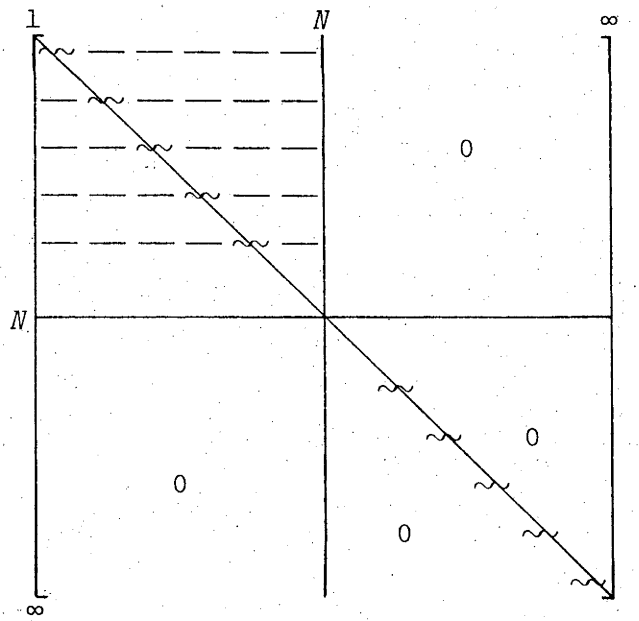
(a)



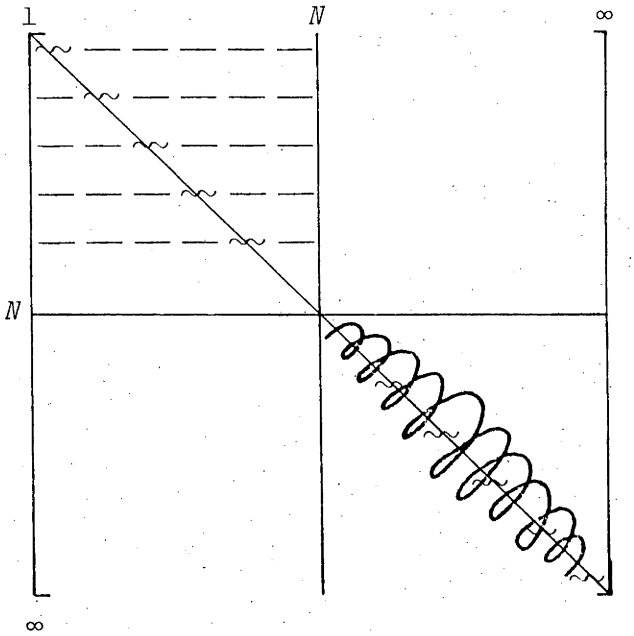
(b)



(c)



(d)



(e)

FIGURE (2.5.1): A schematic view of the matrix D of eq. (2.5.1) in various R-matrix type methods. Figure (a) represents the idealized SRM method in H^{∞}, whereas fig. (b) corresponds to the usual SRM method in H^{N}. The GRM method improves the diagonal and non-diagonal elements in H^{N} [fig. (c)] and the BCRM method [fig. (d)] treats the diagonal part of the interaction exactly in H^{∞} to yield results superior to the SRM method. Figure (e) depicts the situation for the VCRM method in which the wave function of the BCRM method is used as a trial function (εH^{∞}) in the Kohn variational principle to achieve a higher degree of accuracy. Please refer to the text for the explanation of various symbols.

it may even diverge by including distant levels[75].

The necessity for including the effect of distant levels in the SRM method is mainly due to the fact that, for orthogonal (basis) states, the corresponding values of the reduced widths in the H^D space are as large as those in the H^N space and the relative importance of the former declines only as the first inverse power of the energy[50]. Consequently, these levels can combine coherently to influence quite significantly the predictions, e.g., of elastic scattering cross sections(*). Although it is practically impossible to translate H^N into H^∞ fully, Buttle has introduced a method[63] of improving the SRM results. This method, hereafter referred to as the Buttle corrected R-matrix (BCRM) method, partially takes into account the effects of the distant levels in H^∞ by considering the matrix elements of H^∞_d in an analytic way. This is illustrated diagramatically in figure (2.5.1d).

In order to achieve a higher degree of accuracy in cases where the BCRM method may be less effective due to the influence of H^∞_n, one should incorporate the effect of the neglected terms in the overall formulation. This has been done very recently by Heller[91] and Zvijac *et al.*[92] within the framework of the variationally corrected R-matrix (VCRM) method. As pointed out schematically in figure (2.5.1e), they employ an exact solution (e.g. the BCRM method wave function) to an approximate potential in H^∞ as a trial function in the variational formula[99,141] to obtain an improved R-matrix. In other words, the method uses the variational formula for correcting the trial wave function by accounting for the variations resulting from that part of the Hamiltonian in H^∞_n which is not treated in the BCRM

(*) This seems to be the rationale for the overestimate of the elastic forward peak in the SRM calculations mentioned at the end of Section 2.3.

method.

The essence of the BCRM method is the observation that the R-matrix in the SRM method does not reduce to the exact expression for the R-matrix when the coupling interaction in the space H^N is switched off. In other words, for $H_1 = 0$ in eq. (2.3.18); the reduced width amplitudes ζ_{pc} [eq. (2.3.6)] coincide with the amplitudes γ_{pc} [eq. (2.3.14)] of the coupled system to yield an R-matrix, say ${}^0R^N$, corresponding to H_0; viz.

$$ {}^0R^N_{c'c''} = \sum_{p=1}^{N} \zeta_{pc'}\zeta_{pc''}/\left(E_p^{(0)}-E\right) . \qquad (2.5.3) $$

The corresponding exact R-matrix, however, is

$$ {}^0R^\infty_{c'c''} = \sum_{p=1}^{\infty} \zeta_{pc'}\zeta_{pc''}/\left(E_p^{(0)}-E\right) , \qquad (2.5.4) $$

and differs from ${}^0R^N$ by the quantity

$$ {}^0R^D_{c'c''} = \sum_{p=N+1}^{\infty} \zeta_{pc'}\zeta_{pc''}/\left(E_p^{(0)}-E\right) , \qquad (2.5.5) $$

which may be termed the *Buttle correction*.

Thus the Buttle corrected R-matrix should be written in the form

$$ R^B = R + {}^0R^D \qquad (2.5.6) $$

where R is defined through eq. (2.3.13) in H^N space and can be calculated by the SRM method. It is interesting to note that for $H_1 = 0$, $R \to {}^0R^N$ and R^B, therefore, reduces to the correct form ${}^0R^\infty$.

It, therefore, remains to find a calculable form of ${}^0R^D$. In the zero coupling limit this contribution to R^B becomes diagonal in the channel space since, for a fixed p, $\zeta_{pc''}$ has a finite value in only one channel. Consequently, ${}^0R^D_{c'c''}$ may be replaced by ${}^0R^D_{c'c'}$ in the distant space.

Even then it is not possible to calculate this quantity by simply summing over the infinite number of levels in H^D . However, the quantity ${}^0R^\infty$ of eq. (2.5.4) can be calculated exactly by a knowledge of the R-function[18], say, $R^{(0)}_{cc}$ in H^∞ . It can be shown [Appendix (2.5A)] that for an exactly calculable (uncoupled) wave function in a particular channel with

$$(H_0-E)\,|\psi^{(0)}_\lambda\rangle = 0 \ , \tag{2.5.7}$$

this quantity is simply given as

$$R^{(0)}_{cc} = \left\{\left[r\,\frac{d}{dr}\left\{ln\ \psi^{(0)}_{\lambda c}(r)\right\}\right]_{r=a_c} - b_c\right\}^{-1} \ , \tag{2.5.8}$$

where b_c is a fixed number defined in the appendix. Therefore,

$${}^0R^D_{c'c'} = R^{(0)}_{c'c'} - {}^0R^N_{c'c'} \ , \tag{2.5.9}$$

and the calculable form of the Buttle corrected R-matrix can be written as

$$R^B_{c'c''} = R_{c'c''} + {}^0R^D_{c'c'} \ . \tag{2.5.10}$$

The corresponding wave function

$$(\phi_{c'}|\psi^B\rangle = \sum_{c''} R^B_{c'c''}\left[\left\{\frac{d}{dr}\,r-b_{c''}\right\}(\phi_{c''}|\psi^B\rangle\right]_{r=a_{c''}} \ , \tag{2.5.11}$$

is obtained by substituting eq. (2.5.10) in the SRM wave function of eq. (2.3.22) and using the expression (2.3.13) for the corresponding R-matrix. Notice that the arbitrary boundary condition parameter $b_{c''}$ neither affects the wave function nor the S-matrix[18,152,153]. The reason for this is that the dependence of the wave function on $b_{c''}$ is compensated by a similar dependence of $R_{c'c''}$ on this parameter.

Buttle has applied the correction to the $^{12}C(p,\,p')^{12}C$ reaction[63] and found that the results with three levels per channel are not only superior to the equivalent SRM method calculations [discussed at the end of Section 2.3], but are also in very good agreement with the exact coupled-

channels calculations. Later, the BCRM method was applied extensively to atomic and molecular scattering and reactions[154-157]. In these cases the density of states tends to be very large[134,158,159] and hence the need for including the Buttle correction becomes more important than for scattering and reaction problems in nuclear physics. As a matter of fact, the convergence in these cases sometimes requires - even with the BCRM method - a large number of basis states per channel. In such cases the VCRM method[92] has been found to be quite successful for decreasing the size of the basis set at the expense, however, of increased complexity in the overall formulation.

2.6 Summary and discussion

In this chapter several existing methods for estimating the reaction cross sections in the resonant and the non-resonant regions have been discussed. In the original R-matrix theory of Wigner and Eisenbud the configuration space is divided into an internal and an external region. This theory does not incorporate any interaction since, accordingly, the nuclear interaction is assumed to be too complicated to tackle explicitly. For the study of an isolated narrow resonance p, the R-matrix is given in terms of the R-function for channel c:

$$R_{cc}(b_c) = R_B + \gamma_{pc}^2/(E_p - E) \quad , \tag{2.6.1}$$

where the parameters R_B (background contribution which may or may not be zero), γ_{pc} (reduced width amplitude), E_p (resonance energy) together with the boundary conditions b_c (boundary condition parameter) and a_c (channel radius) are used to reproduce the important features of the resonance around energy E. If there are several resonances, say ν, with the same spin and parity, a straightforward generalization of the above

relation i.e.

$$R_{cc}(b_c) = R_B + \sum_{p=1}^{\nu} \gamma_{pc}^2/(E_p - E) \quad , \tag{2.6.2}$$

is often used.

The overall formulation no longer remains so simple when more than one channel is involved. However, as shown in Section 2.2, the complete R-matrix can be derived from a dynamical approach such that

$$\begin{aligned} R_{cc'}(b_c) &= \sum_{p=1}^{\infty} \gamma_{pc}\gamma_{pc'}/(E_p - E) \\ &= \sum_{pq} \gamma_{pc}(A^{-1})_{pq}\gamma_{qc'} \\ &= R_B + \sum_{p=1}^{\nu} \gamma_{pc}\gamma_{pc'}/(E_p - E) \quad , \end{aligned} \tag{2.6.3}$$

where the elements of the level-matrix A are given by eq. (2.2.31) and the remaining symbols have their usual significance. In order to determine the cross sections of any particular reaction from the above, one has to determine the appropriate values of the necessary parameters from the corresponding experimental data and to calculate the R- and S-matrices, respectively, through the relations (2.6.3) and (2.2.45) or (2.2.46).

The main drawback of using the R-matrix theory is that most of the parameters involved do not have any particular physical significance. The SRM method, on the other hand, enables one to predict the cross section of a given reaction from a definite nuclear model in a coherent way. In principle, the eigenstates of the total Hamiltonian H $(\equiv H_0 + \Delta H)$ are expanded in terms of a complete set of basis states $|p, c\rangle$. The latter are eigenfunctions of the model Hamiltonian H_0 in each channel within the internal region, where all the channels are coupled through a residual interaction ΔH . This differs significantly from the equivalent situation in the R-matrix theory. The corresponding R-matrix is determined by

adopting the diagonalization procedure described in detail in Section 2.3 for a truncated basis set. In this spirit the method may be considered as an alternative procedure for solving the coupled-channels problems in nuclear, atomic and molecular physics. However, it has been found that in some cases a large number of basis states is required in order to achieve satisfactorily converged results.

Two methods of overcoming the poor convergence of the SRM method have been developed. The first is the GRM method [Section 2.4] which essentially uses a more general form of basis states satisfying inhomogeneous boundary conditions at the surface of the internal region. The second approach is to try to include the infinite basis set corresponding to the model Hamiltonian H_0 exactly in the infinite dimensional Hilbert space. The BCRM method [Section 2.5] may be considered as the first successful step in this direction(*). The results so obtained may be improved further by taking into account the VCRM method in which the variational principle is used for correcting the BCRM method wave function or phase shifts in the complete Hilbert space.

In conclusion, the R-matrix type methods discussed so far are quite suitable for predicting the main features of the reaction cross sections when a suitable nuclear model is available. Each method, however, has some advantages as well as some problems. The latter implies that there is still a need for further development and research; especially if further details of the reaction cross sections are to be reproduced with a *desirable* accuracy in the overall formulation.

(*) Another method incorporating an infinite basis set is the Jacobi matrix method of Heller and Yamani[160,161]. The method employs fixed exponent Laguerre or Hermite basis functions for the operator $H_0 = -\frac{1}{2} d^2/dr^2$ and may be regarded as the generalization of the SRM method in the sense of Feshbach[77-79]. In view of its limited applications to atomic scattering problems together with the restrictions due to the employment of basis functions which are not scattering functions, this method may not be very successful in nuclear scattering and reaction problems.

CHAPTER 3

NATURAL BOUNDARY CONDITION METHODS

3.1 Introduction

The present chapter is devoted to the study and development of two new R-matrix type methods for estimating reaction cross sections. Keeping in mind the hierarchy of methods discussed in the preceding chapter, one may question the need for developing any new method. In this connection it may be worth emphasizing that the search for new methods should not be relinquished until one has found a method which is as accurate as desired, numerically fast, requires a minimum of computer storage and can be generalized to more complicated systems in a straightforward manner.

As stated earlier, the R-matrix type methods deal with the scattering or reaction of an incident particle with a target nucleus through the formation of an intermediate state. One way of understanding the behaviour of the overall system is to analyse the process which mixes the characteristics of the incident particle with those of the target. Within the framework of the SRM method, this "configuration mixing" is usually established through the operators ΔH (residual interaction) and ΔL (boundary condition mixing) in a definite way. Previous studies with different R-matrix type methods have revealed that each method depends heavily on the choice of these quantities. Whereas the BCRM and the VCRM methods basically concentrate on accounting for the effects of a large ΔH, the GRM method mainly takes into consideration the effects of a variation in ΔL explicitly. On the other hand, the development of the natural boundary condition (NBC) methods is based on the speculation that an optimum choice of boundary condition parameters (e.g. $\Delta L = 0$) together with the most realistic model for the single particle potential (i.e. ΔH = minimum) should minimize the number of basis states for achieving a desirable

accuracy. This is equally important for applications in atomic or molecular physics[154-161] in which the number of reaction channels is large.

Starting from a description of what is meant by natural boundary conditions in the present context (Section 3.2), the Barrett and Delsanto (BD) method is briefly discussed in Section 3.3. The formulation of the iterative R-matrix (IRM) method for one open channel is developed in subsection 3.4.1 whereas the following subsection deals with the extension of the method to more than one open channel. A simple correction to the BD method which can greatly improve the rate of convergence is described in Section 3.5.

3.2 The Natural Boundary Conditions

For simplicity consider the scattering of a neutral particle with energy E, in the centre of mass system, from a central potential V. The total (physical) wave function ψ of the system is such that

$$(T+V+L(b)-E)\psi = L(b)\psi \ , \qquad (3.2.1)$$

where T is the kinetic energy operator and $L(b)$ is the single channel analogue of the Bloch operator defined in the previous chapter. Within the framework of the SRM method, the physical wave function obeys the boundary condition $L(b)\psi = 0$ at the matching radius $r = a$. Consequently the energy-dependent boundary condition parameter may be written as

$$b \equiv f(E) = \left[r \frac{d}{dr} \{ln\ u_l(r)\} \right]_{r=a} , \qquad (3.2.2)$$

where $u_l(r)$ is the radial part of the physical wave function for orbital angular momentum l.

In the internal region, the wave function ψ can be expanded as usual, viz.

$$\psi = \sum_{\lambda=1}^{\infty} C_\lambda V_\lambda \ , \qquad (3.2.3)$$

where the basis states V_λ are such that

$$\left(T+V+L(\tilde{b})-E_\lambda\right)V_\lambda = L(\tilde{b})V_\lambda \ . \qquad (3.2.4)$$

The boundary condition parameters $\tilde{b}$ are usually arbitrary, but in the present case the V_λ are chosen such that $L(\tilde{b})V_\lambda = 0$; i.e.

$$\tilde{b} = \left[r \frac{d}{dr} \{ln\ V_{\lambda l}(r)\}\right]_{r=a} \ . \qquad (3.2.5)$$

At this point one may think about minimizing the number of terms in the series (3.2.3) without abruptly truncating it to any finite number. The *natural* way is to try to use the *characteristics* of the physical wave function in defining the wave function V_λ in the internal region. A comparison of equations (3.2.5) and (3.2.2) shows that whenever $b = \tilde{b}$, i.e. as ΔL [$\equiv L(b)-L(\tilde{b})$] vanishes, $V_{\lambda l}(r) \to U_l(r)$. This defines the natural boundary condition for the system and the value of $\tilde{b}$ for which the condition $\Delta L = 0$ holds identically, at $E_\lambda = E$, will be called the natural boundary condition (n.b.c.) parameter for the basis state V_λ . In a similar way one can define the physical n.b.c. parameter corresponding to the physical wave function ψ .

In the single channel (potential) scattering case the advantage of the n.b.c. parameters is the representation of the physical wave function within the internal region by only one term of the infinite series (i.e. by the total wave function itself). It can be shown that under these conditions the infinite series in the corresponding R-function [eq. (2.5A.6)] reduces to only one term at $E = E_\lambda$. It may be worth emphasizing that the n.b.c.

parameters defined here differ significantly(*) from the definitions given by Buttle[63] (i.e. $\tilde{b} = -l$ or zero) and resemble very much those defined by Danos and Greiner[107] and Zvijac *et al*[92]. In this case the n.b.c. parameters are real, unknown and energy-dependent and the method of their estimation will be discussed fully in the following sections.

The natural boundary condition parameters no longer remain simple for cases involving more than one channel. Because of the coupling to and between other channels, one may need more than one basis state per channel for achieving a desirable accuracy. Furthermore, the n.b.c. parameters

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(*) The concept of natural boundary conditions was first introduced by Siegert[162] in deriving the Kapur-Peierls dispersion formula[30] from a different viewpoint. Teichmann[163,164], on the other hand has investigated the characteristics of the corresponding *R*-matrix in a detailed discussion regarding the general properties of the cross sections appearing in the dispersion theory of nuclear reactions[32-34]. He has also exploited the importance of similar boundary conditions in establishing some formal connections[165] between the effective range formula and the *R*-matrix theory of Wigner and Eisenbud. Teichmann and Wigner[166] appear to have been the first to discuss the energy dependence of some natural boundary condition parameters. Their approach turned out to be quite useful in simplifying the sum rules in dispersion theory. Bohr and Mottelson[76] have also discussed a similar energy variation of a boundary condition like quantity within the framework of a reaction theory formulated on the basis of coupling between individual particle and collective features of the target nucleus.

Later, Peierls[38], Le Couteur[39], Humblet and Rosenfeld[40] used natural boundary conditions in different contexts of formal reaction theories. Vogt[22] has defined his n.b.c. parameters as the shift function[18] at the resonance energy in an *R*-matrix type treatment of neutron-nucleus reactions. The present n.b.c. concept was extensively utilized in the eigenchannel method for nuclear reactions[93,96].

Lejeune and Mahaux[167] have discussed the importance of n.b.c. parameters in the one-level approximation of *R*-matrix theory for a soluble model. Westin and Adams[168] found similar n.b.c. parameters very useful in predicting fairly accurately the spectroscopic factors for the broad and narrow resonances occurring in the $^{12}C(n, n)^{12}C$ and $^{16}O(n, n)^{16}O$ reactions using *R*-matrix theory. Recently, Vitturi and Zardi[169] have also used some typical n.b.c. parameters for simplifying the general framework for nuclear resonance theories in terms of the Bloch formalism.

become complex and hence require a special treatment. However, it should be emphasized that this problem exists only for open channels. For closed channels, the n.b.c. parameters are real and known(*), being given by eq. (3.2.5) with $V_{\lambda l}(r)$ replaced by an exponentially decaying outgoing wave function[18] in the appropriate channel at the desired energy.

3.3 Barrett and Delsanto Method

The Barrett and Delsanto (BD) method is essentially a generalization of an approach which was suggested by Danos and Greiner[107] for the single channel case and eventually abandoned in favour of the first of the NBC methods i.e. the eigenchannel (EC) method. The EC method basically utilizes a matrix diagonalization technique and is easily extendable to more complicated systems with sophisticated nuclear models. Unfortunately, this method is extremely time consuming since it involves many diagonalizations of large matrices. While retaining the flexibility of the diagonalization of the EC method, the main aim of developing the BD method[108] was to eliminate these numerical deficiencies and hence to drastically reduce the computing time involved.

In this method the configuration space is divided into internal and external regions, the surfaces of the boundaries being defined by channel radii $r_c = a_c$ as in the SRM method. For simplicity it is assumed that all the channel radii have the same value i.e. $a_c = a$ and the surface function $|\phi_c)$ as defined in eq. (2.2.40) is denoted by $|c)$.

Using the Bloch operator

$$L(b_c) = \sum_c |c) \frac{\hbar^2}{2\mu_c} \delta(r_c - a) \left[\frac{d}{dr_c} - \frac{b_c - 1}{a}\right] (c| \ , \qquad (3.3.1)$$

(*) In a strict sense these parameters are known provided that the corresponding threshold energy is given.

in the notation of Lane and Robson[48], the Schrödinger equation

$$(H-E_i)\psi_i = (H_0+H_1-E_i)\psi_i = 0 \ , \qquad (3.3.2)$$

may be written for the internal region $r_c \le a$ in the form

$$(H+L(b_c)-E_i)\psi_i = L(b_c)\psi_i \ . \qquad (3.3.3)$$

The wave function ψ_i may be expanded in terms of a complete set of basis states ϕ_j which are regular at the origin and satisfy the equation

$$H_0\phi_j = \varepsilon_j\phi_j \ , \qquad (3.3.4)$$

with the boundary conditions

$$L(b_c)\phi_j = 0 \ , \text{ for } r_c = a \ . \qquad (3.3.5)$$

Writing

$$\psi_i = \sum_j a_{ij}\phi_j \ , \qquad (3.3.6)$$

one obtains the infinite set of equations

$$\sum_j a_{ij}\left[(\varepsilon_j-E_i)\delta_{kj}+V_{kj}\right] = \langle \phi_k | L(b_c)\psi_i \rangle \ , \qquad (3.3.7)$$

where $V_{kj} = \langle \phi_k | H_1 | \phi_j \rangle$, $\langle \phi_k | \phi_j \rangle = \delta_{kj}$ and the angular brackets denote integration over the internal region.

If the condition

$$L(b_c)\psi_i = 0 \ , \text{ for } r_c = a \ , \qquad (3.3.8)$$

is satisfied, the quantities b_c are defined to be natural boundary condition parameters for the wave function ψ_i . In practice, the infinite sum in eq. (3.3.6) is truncated at $j = \sum_c N_c = \nu$ say, where N_c is the number of radial quantum numbers kept for each channel c . For simplicity it is assumed that $N_c = N$ for all c . Thus for n.b.c. parameters eq. (3.3.7) reduces to the finite set of equations

$$\sum_{j=1}^{\nu} a_{ij}\left[(\varepsilon_j-E_i)\delta_{kj}+V_{kj}\right] = 0 \ , \qquad (3.3.9)$$

which has non-zero solutions for the coefficients a_{ij} only if

$$\det\left[(\varepsilon_j - E_i)\delta_{kj} + V_{kj}\right] = 0 \ . \qquad (3.3.10)$$

The solutions of eq. (3.3.10) are the eigenvalues E_i of the Schrödinger equation although in general none of the E_i are equal to the excitation energy E_x of the nuclear system.

For closed channels, the physical n.b.c. parameters are "real" and "known" being given by

$$(b_c)_{\text{closed}} = \left[r_c O_c'/O_c\right]_{r_c=a} \ , \qquad (3.3.11)$$

where O_c is the exponentially decaying outgoing particle radial wave function for channel c and the prime represents radial differentiation.

For the case of only one open channel, the physical n.b.c. parameter is also "real" and is defined by

$$(b_c)_{\text{open}} = \left[r_c \frac{F_c'\cos\delta_c + G_c'\sin\delta_c}{F_c\cos\delta_c + G_c\sin\delta_c}\right]_{r_c=a} \ , \qquad (3.3.12)$$

where F_c and G_c are the regular and irregular solutions of the radial differential equation and δ_c is the phase shift. Of course, δ_c (and hence b_c) is not known *a priori*. The general procedure is to adjust b_c so that one of the eigenvalues $E_i = E_x$ when the corresponding δ_c determines the cross section.

For several open channels, M, the physical n.b.c. parameters are complex and unsuitable for defining basis states. In this case, there are M wave functions ψ_k with an eigenvalue $E_i = E_x$ and which for $r_c \geq a$ satisfy

$$\psi_k = \sum_c \left[I_c\delta_{kc} - S_{kc}O_c\right] \ , \quad k = 1, 2, \ldots, M \ , \qquad (3.3.13)$$

where S_{kc} is a usual S-matrix element and the quantities I_c and O_c

are defined explicitly in eqs. (2.2.38) and (2.2.39). It is convenient to transform this set of wave functions into standing wave solutions for $r_c \geq a$,

$$\chi_{k'} = \sum_k (T^-)_{k'k}\psi_k \ , \tag{3.3.14}$$

where

$$T^-_{k'k} = V_{k'k}e^{-i\delta_{k'k}} \tag{3.3.15}$$

and the amplitudes $V_{k'k}$ and the phases $\delta_{k'k}$ are real quantities. Then

$$\chi_{k'} = \sum_{kc} \left[(T^-)_{k'k}I_c\delta_{kc} - (T^-)_{k'k}S_{kc}O_c\right] \ , \tag{3.3.16}$$

which may be written as

$$\chi_{k'} = \sum_k \left[(T^-)_{k'c}I_c - (T^+)_{k'c}O_c\right] \ , \tag{3.3.17}$$

where $(T^+)_{k'k} = V_{k'k}e^{i\delta_{k'k}}$ so that

$$\chi_{k'} = \sum_c V_{k'c}\left[e^{-i\delta_{k'c}}I_c - e^{i\delta_{k'c}}O_c\right] \ , \tag{3.3.18}$$

and

$$S_{kc} = \sum_{k'} \left[(T^-)^{-1}\right]_{kk'}(T^+)_{k'c} \ . \tag{3.3.19}$$

The standing wave solutions $\chi_{k'}$ have real n.b.c. parameters

$$b_c^{(k')} = \left[r_c \frac{F'_c\cos\delta_{k'c} + G'_c\sin\delta_{k'c}}{F_c\cos\delta_{k'c} + G_c\sin\delta_{k'c}}\right]_{r_c=a} \ . \tag{3.3.20}$$

In order to obtain the S-matrix, the procedure is as follows. The known n.b.c. parameters for the closed channels and arbitrary values of the $b_c^{(k')}$ (and hence $\delta_{k'c}$) for all except one of the open channels are used. The remaining $b_c^{(k')}$ is varied until one of the eigenvalues $E_i = E_x$ and following the method described in detail in the Appendix (3.3A), the

coefficients a_{ij} are determined for each value of k' . In each case, the phases $\delta_{k'c}$ are given in terms of the $b_c^{(k')}$ by eq. (3.3.20) and the amplitudes $V_{k'c}$ may be obtained by matching the internal and external wave functions at $r_c = a$. From a knowledge of the matrix elements $(T^{\pm})_{k'c}$, the S-matrix is then given by eq. (3.3.19).

3.4 Iterative R-matrix Method

The iterative R-matrix (IRM) method resembles the BD method in the sense that both employ basis states which satisfy natural boundary conditions. The main difference, however, is in the numerical techniques, i.e. the BD method employs "matrix diagonalization" whereas the IRM method uses "matrix inversion" for determining the physical solutions of the nuclear Schrödinger equation. The IRM method may also be regarded as a variant of the SRM method. Its typical characteristics, however, are the incorporation of an energy-dependent basis chosen by an iterative procedure and the employment of a matrix inversion technique.

Since the physical n.b.c. parameters are real for one open channel and complex for more than one open channel, the development of the IRM method is divided into two parts: subsections 3.4.1 and 3.4.2, respectively.

3.4.1 ONE OPEN CHANNEL

Assuming that the fundamental assumptions of the SRM method together with the necessary simplifications discussed at the beginning of the BD method (Section 3.3) hold; the Schrödinger equation for the system may be written as

$$(H-E_i)\psi_i = 0 \ , \qquad (3.4.1)$$

where the symbols and notations have the same significance as in the BD method. The wave function for $E_i = E_x$ is given for $r_c \leq a$ by

$$\psi_x = \left(H+L(b_c)-E_x\right)^{-1}L(b_c)\psi_x \ , \qquad (3.4.2)$$

where use has been made of the relations (3.3.1) and (3.3.3) and the parameters b_c are arbitrary although for n.b.c. values the R.H.S. of the equation is indeterminate. For simplicity one may take $b_c = 0$ so that

$$\begin{aligned}\psi_x &= \left(H+L(0)-E_x\right)^{-1}L(0)\psi_x \\ &= \sum_{jj'} |\phi_j\rangle\left(A^{-1}\right)_{jj'}\langle\phi_{j'}|L(0)|\psi_x\rangle \ , \end{aligned} \qquad (3.4.3)$$

where the basis states satisfy the equations

$$H_0\phi_j = \varepsilon_j\phi_j \ , \qquad (3.4.4)$$

$$L(b_c)\phi_j = 0 \ , \qquad (3.4.5)$$

with the parameters b_c as yet unspecified and

$$\begin{aligned}A_{jj'} &= \langle\phi_j|H_0+H_1+L(0)-E_x|\phi_{j'}\rangle \\ &= \left[\left(\varepsilon_j-E_x\right)\delta_{jj'}+\langle\phi_j|L(0)|\phi_{j'}\rangle+V_{jj'}\right] . \end{aligned} \qquad (3.4.6)$$

For the external region $r_c \geq a$,

$$\psi_x = \sum_{c'} \left[I_{c'}\delta_{cc'}-S_{cc'}O_{c'}\right] , \qquad (3.4.7)$$

where c defines the incident channel and the remaining symbols have their usual significance. Matching the internal and external solutions ψ_x at $r_c = a$ and projecting on to the surface function $(c'|$ gives the set of coupled equations

$$\left[\tilde{I}_c\delta_{cc'}-S_{cc'}\tilde{O}_{c'}\right] = \sum_{c''} R_{c'c''}\left[\left(r_{c''}\tilde{I}_{c''}\right)'-S_{cc''}\left(r_{c''}\tilde{O}_{c''}\right)'\right] \ , \qquad (3.4.8)$$

with the R-matrix elements

$$R_{c'c''} = \frac{\hbar^2 a}{2\mu_{c''}} \sum_{jj'} (c'|\phi_j\rangle\left(A^{-1}\right)_{jj'}\langle\phi_{j'}|c'') \ , \qquad (3.4.9)$$

where the quantities $(c'|\phi_j\rangle$ are radial functions at $r_{c'} = a$ and $\tilde{I}_c$ and $\tilde{O}_c$ are unit flux incoming and outgoing radial functions. Notice that

for $b_c \neq 0$ in eq. (3.4.3), the above set of coupled equations assumes a form similar to eq. (2.3.21).

The S-matrix elements may be determined by solving the coupled equations for a sufficiently complete set of energy-independent basis states ϕ_j. This is essentially the SRM method using a matrix inversion technique, which for some cases may require a large number of basis states. In order to keep the number of basis states to a minimum the following procedure is suggested.

The basic idea is to use n.b.c. parameters to define the basis states. For the case of only one open channel, all the physical n.b.c. parameters are real and are given by eqs. (3.3.11) and (3.3.12). Only for the incident (open) channel is the n.b.c. parameter not known. For this channel (c), an arbitrary value of b_c (say 0) may be employed together with the physical n.b.c. parameters for the closed channels to define a more severely truncated set of basis states than would be required for convergence in a SRM calculation with energy-independent basis states. Using this basis the S-matrix may be obtained from eq. (3.4.8). A new value of b_c may then be determined from eq. (3.3.12) since

$$S_{cc} = e^{2i\delta_c}, \tag{3.4.10}$$

and the calculation repeated with new basis states for the open channel. This defines an iterative procedure which in general converges to the result obtained by the BD method. The method requires a slight modification for energy regions where $|b_c|$ is very large corresponding to vanishingly small R-matrix elements. This point will be discussed further in the next subsection.

3.4.2 SEVERAL OPEN CHANNELS

As discussed in the last subsection, the physical n.b.c. parameters

b_c , defined by the relation

$$L(b_c)\psi_x = 0 \quad \text{for} \quad r_c = a \ , \tag{3.4.11}$$

are real for the case in which only one channel is open. For the incident (open) channel the n.b.c. value may be determined by the iterative procedure, the n.b.c. parameters being known for any closed channels. For M (> 1) open channels the physical n.b.c. parameters are complex and unsuitable for defining basis states. Furthermore, there are M degenerate wave functions ψ_k satisfying the Schrödinger equation at energy E_x . For $r_c \geq a$, these wave functions are of the form

$$\psi_k = \sum_{\tilde{c}} \left[I_{\tilde{c}}\delta_{k\tilde{c}} - S_{k\tilde{c}}O_{\tilde{c}}\right] - \sum_{\bar{c}} S_{k\bar{c}}O_{\bar{c}} \ ; \quad k = 1, 2, \ldots, M \ , \tag{3.4.12}$$

where $\tilde{c}$ ($\bar{c}$) denotes open (closed) channels, $S_{k\tilde{c}}$, $S_{k\bar{c}}$ are usual S-matrix elements, $I_{\tilde{c}}$ $(O_{\tilde{c}})$ describe unit flux incoming (outgoing) particle waves and the target (residual) nucleus and $O_{\bar{c}}$ represents an exponentially decaying outgoing particle wave and the residual nucleus. Following the BD method, it is convenient to transform this set of wave functions into ones with standing wave solutions for the open channels for $r_{\tilde{c}} \geq a$,

$$\begin{aligned} \chi_{k'} &= \sum_{k} (T^-)_{k'k}\psi_k \\ &= \sum_{\tilde{c}} \left[(T^-)_{k'\tilde{c}}I_{\tilde{c}} - (T^+)_{k'\tilde{c}}O_{\tilde{c}}\right] - \sum_{\bar{c}} (F^-)_{k'\bar{c}}O_{\bar{c}} \ , \end{aligned} \tag{3.4.13}$$

where

$$(T^{\pm})_{k'k} = V_{k'k}e^{\pm i\delta_{k'k}} \ , \tag{3.4.14}$$

$$(F^-)_{k'\bar{c}} = \sum_{k} (T^-)_{k'k}S_{k\bar{c}} \ , \tag{3.4.15}$$

$$S_{k\tilde{c}} = \sum_{k''} \left[(T^-)^{-1}\right]_{kk''}(T^+)_{k''\tilde{c}} \ , \tag{3.4.16}$$

and $V_{k'k}$ $(\delta_{k'k})$ represent the corresponding amplitudes (phases).

The wave functions $\chi_{k'}$ have real n.b.c. parameters $b_{\tilde{c}}^{(k')}$ [e.g. eq. (3.3.20)] for the open channels as well as for the closed channels. Application of the transformation (3.4.13) to eq. (3.4.8) of the previous subsection results in the following set of equations

$$\left[(T^-)_{k'\tilde{c}},\tilde{I}_{\tilde{c}},-(T^+)_{k'\tilde{c}},\tilde{O}_{\tilde{c}},\right] = \sum_{\tilde{c}''} R_{\tilde{c}',\tilde{c}''}\left[(T^-)_{k'\tilde{c}''}(r_{\tilde{c}''}\tilde{I}_{\tilde{c}''})'-(T^+)_{k'\tilde{c}''}(r_{\tilde{c}''}\tilde{O}_{\tilde{c}''})'\right]$$

$$- \sum_{\bar{c}''} R_{\bar{c}',\bar{c}''}(F^-)_{k'\bar{c}''}(r_{\bar{c}''}\tilde{O}_{\bar{c}''})' ,$$

$$-(F^-)_{k'\bar{c}},\tilde{O}_{\bar{c}'} = \sum_{\tilde{c}''} R_{\bar{c}',\tilde{c}''}\left[(T^-)_{k'\tilde{c}''}(r_{\tilde{c}''}\tilde{I}_{\tilde{c}''})'-(T^+)_{k'\tilde{c}''}(r_{\tilde{c}''}\tilde{O}_{\tilde{c}''})'\right]$$

$$- \sum_{\bar{c}''} R_{\bar{c}',\bar{c}''}(F^-)_{k'\bar{c}''}(r_{\bar{c}''}\tilde{O}_{\bar{c}''})' , \quad (3.4.17)$$

where the R-matrix elements are unchanged and defined by eq. (3.4.9).

The S-matrix elements $S_{k\tilde{c}}$, and hence the cross sections, may be determined in the following manner. The known n.b.c. parameters for the closed channels, arbitrary values of the $b_{\tilde{c}''}^{(k')}$ (and hence of the phase shifts $\delta_{k'\tilde{c}''}$) for all except one of the open channels k', together with an initial guess for the value of $b_{k'}^{(k')}$ are used to construct a finite set of basis states (N levels/channel). The R-matrix elements are calculated in this basis and the coupled equations (3.4.17) solved to obtain the remaining phase shift $\delta_{k'k'}$ (as well as the M-1 relative amplitudes $V_{k'\tilde{c}''}/V_{k'k'}$). From this derived value of $\delta_{k'k''}$, a new value of $b_{k'}^{(k')}$ may be obtained using eq. (3.3.20) and the calculations repeated with new basis states for the channel k'. This defines an iteration procedure which in general converges to the result obtained by the BD method. The procedure has to be repeated M times corresponding to a different choice

of the open channel k' for which $b_{k'}^{(k')}$ is varied. In this way the matrix elements $(T^{\pm})_{k'\tilde{c}'}$ are obtained and the S-matrix determined from eq. (3.4.16).

As indicated in the previous subsection, for some excitation energies the IRM method does not necessarily converge to the result of the BD method. If during the iteration process the boundary condition being varied, $b_{k'}^{(k')}$, becomes large (say $|b_{k'}^{(k')}| > 100$), the method often converges to a value of $|b_{k'}^{(k')}| \to \infty$ and not to the n.b.c. value. This problem is readily overcome by employing a better initial guess (e.g. based upon knowledge of the n.b.c. value at the neighbouring excitation energies) for the parameters $b_{k'}^{(k')}$.

Unlike the SRM and BCRM methods, the NBC methods do not lead automatically to an exactly symmetric and unitary S-matrix for the case of several open channels. However, an *exactly* symmetric and unitary S-matrix can be obtained by the unitarization procedure described in the Appendix (3.4A). The elements of the S-matrix so obtained may be used for calculating the reaction cross sections. In practice the lack of symmetry in the S-matrix resulting from eq. (3.4.16) is a distinct advantage since it gives an indication of the overall error in the calculation using a given truncated basis set. Another test which can be used to check the convergence of the NBC methods is that the quantity $(T^{-})(T^{-})^{+}$ should be real.

3.5 Energy Correction to the BD Method

Consider a situation in which the BD method has been strictly followed with a basis truncated to N levels in each channel. Assume that the iteration of the boundary condition parameter on one channel has

been computed and that natural boundary conditions now apply such that one of the eigenvalues, E_i, of the energy matrix is equal to the excitation energy E_x. The eigenfunction ψ_i, associated with the eigenvalue E_i, can be expanded in terms of the basis states, ϕ_j,

$$\psi_i = \sum_j a_{ij}\phi_j \ . \tag{3.5.1}$$

The secular equation [i.e. eq. (3.3.9)] may be written

$$\sum_j a_{ij}\langle\phi_k|H|\phi_j\rangle = \langle\phi_k|H|\psi_i\rangle = E_i a_{ik} \tag{3.5.2}$$

and can be solved in the usual way to yield the eigenvalues, E_i, and the coefficients a_{ij}.

In order to investigate the effect of including a previously neglected level, ϕ_m, one may consider that the addition of this level modifies eq. (3.5.1) for the wave function, which is now given by

$$\bar{\psi}_i = \sum_j b_{ij}\phi_j + b_{im}\phi_m \ . \tag{3.5.3}$$

The sum in the above equation (and in subsequent equations) runs over only those levels, ϕ_j, which are treated exactly, the extra level, ϕ_m, being written explicitly.

The secular equation now becomes:

$$\sum_j b_{ij}\langle\phi_k|H|\phi_j\rangle + b_{im}\langle\phi_k|H|\phi_m\rangle = \bar{E}_i b_{ik} \ , \tag{3.5.4'}$$

$$\sum_j b_{ij}\langle\phi_m|H|\phi_j\rangle + b_{im}\langle\phi_m|H|\phi_m\rangle = \bar{E}_i b_{im} \ , \tag{3.5.4"}$$

where $\bar{E}_i$ are the new eigenvalues, which have been slightly shifted from the old values, E_i, by the introduction of the extra level. Defining Z_{il} by the relationship

$$Z_{il} \equiv \sum_j b_{ij} a_{lj} \ , \tag{3.5.5}$$

so that

$$b_{ij} = \sum_l a_{lj} Z_{il} \ , \tag{3.5.6}$$

since the coefficients a_{lj} are the elements of an orthogonal matrix and using eq. (3.5.2), one may rewrite eqs. (3.5.4) in the form:

$$E_l Z_{il} + b_{im} \langle \psi_l | H | \phi_m \rangle = \overline{E}_i Z_{il} \ , \tag{3.5.7'}$$

$$\sum_l Z_{il} \langle \phi_m | H | \psi_l \rangle + b_{im} \langle \phi_m | H | \phi_m \rangle = \overline{E}_i b_{im} \ . \tag{3.5.7"}$$

Rearrangement of eq. (3.5.7') yields

$$Z_{il} = b_{im} \langle \psi_l | H | \phi_m \rangle / (\overline{E}_i - E_l) \ , \tag{3.5.8}$$

which upon substitution into eq. (3.5.7") gives

$$\overline{E}_i = \langle \phi_m | H | \phi_m \rangle + \sum_l \frac{| \langle \psi_l | H | \phi_m \rangle |^2}{\overline{E}_i - E_l} \ . \tag{3.5.9}$$

As one is only interested in the eigenvalue, $\overline{E}_i$, which is closest to the original eigenvalue $E_i = E_x$, one term is expected to dominate the sum in eq. (3.5.9), i.e.

$$\overline{E}_i \approx \langle \phi_m | H | \phi_m \rangle + \frac{| \langle \psi_i | H | \phi_m \rangle |^2}{(\overline{E}_i - E_i)} \ . \tag{3.5.10}$$

The solution of this equation for $\overline{E}_i$ is

$$\overline{E}_i = \tfrac{1}{2} \left\{ \langle \phi_m | H | \phi_m \rangle + E_i \pm \left[(\langle \phi_m | H | \phi_m \rangle - E_i)^2 + 4 | \langle \phi_m | H | \psi_i \rangle |^2 \right]^{\frac{1}{2}} \right\} \ . \tag{3.5.11}$$

Assuming $| \langle \phi_m | H | \psi_i \rangle | \ll (\langle \phi_m | H | \phi_m \rangle - E_i)$ and expanding the square root by the binomial theorem, the solution for $\overline{E}_i$ near E_i is given by

$$\overline{E}_i \approx E_i - \frac{| \langle \phi_m | H | \psi_i \rangle |^2}{\langle \phi_m | H | \phi_m \rangle - E_i} \ . \tag{3.5.12}$$

The effect of as many higher levels as necessary may be approximately included by successive application of eq. (3.5.12) without increasing the dimensions of the matrices to be diagonalized, and thus without a substantial effect on the computation time. The iteration procedure in the BD method is now allowed to proceed until the corrected value of one of the eigenvalues, $\overline{E}_i$, is equal to E_x. The small correction to the energy results in slightly different values for the natural boundary conditions and thus for the phase shifts in the asymptotic region, δ_{kc}, obtained by matching the internal and external logarithmic derivatives of the wave functions at the channel radii[108].

The expansion coefficients, b_{ij} and b_{im}, in eq. (3.5.3) must also be determined in order to obtain more accurate values for the amplitudes, V_{kc}, of the wave functions in the asymptotic region using, for example, eqs. (2.14) and (2.19) of ref.[108]. From eqs. (3.5.6) and (3.5.8) and assuming $\overline{E}_i \approx E_i$,

$$b_{ij} = b_{im} \sum_l a_{lj} \frac{\langle \psi_l | H | \phi_m \rangle}{\overline{E}_i - E_l} , \tag{3.5.13}$$

$$\approx b_{im} a_{ij} \frac{\langle \psi_i | H | \phi_m \rangle}{\overline{E}_i - E_i} . \tag{3.5.14}$$

Since the normalization is arbitrary, it is convenient to choose

$$b_{im} = \frac{\overline{E}_i - E_i}{\langle \psi_i | H | \phi_m \rangle} \tag{3.5.15}$$

so that

$$b_{ij} = a_{ij} . \tag{3.5.16}$$

The expansion coefficients, b_{ij}, for the components of the wave function treated exactly are thus unchanged by the correction, and the coefficient for the additional component is given approximately by

eq. (3.5.15). These coefficients may be employed to yield improved estimates of the amplitudes, V_{kc}, and hence of the S-matrix and associated reaction cross sections.

3.6 Discussion

The calculation of reaction and scattering cross sections from an assumed underlying physical model is an important part of atomic, molecular and nuclear physics. In principle, the calculation can be performed by the straightforward solution of the coupled integro-differential equations associated with the physical model, but this method is cumbersome when the model is sophisticated. For this reason considerable attention has been given in recent years to alternative approaches to the problem. It has been discussed in detail in the previous chapter that many of these approaches are connected in one way or another with the R-matrix theory of nuclear reactions.

The present chapter has dealt with a detailed study and development of two new (NBC) methods. Both methods involve an iteration procedure in which the boundary conditions applied to the basis states are varied systematically until convergence to an optimum set of natural boundary conditions is achieved. The S-matrix and associated cross sections are calculated using the n.b.c. parameters. In view of the fact that such a choice of boundary conditions requires the minimum number of basis states for a given model Hamiltonian, it is believed that in general both methods, which are closely related, should be very useful for problems in which the number of channels is large. This is a real advantage, for example, over the SRM method which involves energy-independent basis states satisfying arbitrary boundary conditions.

The employment of n.b.c. parameters has the further advantage that at each energy, the convergence criterion of Philpott and George for the GRM

method[75] is automatically satisfied for any channel radii for which there are no polarizing interactions in the external region of configuration space. The main disadvantage is that the n.b.c. basis states are energy dependent which implies that most of the computing time is taken up in calculating these basis states. This means that this part of the computer code should be highly efficient.

Amongst other methods discussed in detail in the previous chapter, the BCRM method[63] has been quite successful in applications to several reaction problems. Zvijac *et al.*[91,92] have investigated an extension of the BCRM method by the inclusion of an extra variational correction. In comparing these methods with the NBC methods, it should be noted that Zvijac *et al.* claim that both the Buttle correction and their variational correction are zero when n.b.c. parameters are used. In other words, the NBC methods are automatically Buttle corrected and variationally corrected. The energy correction to the BD method thus represents an additional improvement.

Before concluding this chapter, it may be worth emphasizing that the present year (1976) has been quite productive in connection with the development of new and sophisticated methods for the efficient calculation of cross sections. Recently, Nordholm and Bacskay have demonstrated how to apply the generalized finite element (GFE) method to the bound and continuum state calculations[170,171]. The GFE method is essentially a particular choice of basis functions e.g. instead of using traditional eigenfunctions of some model Hamiltonian which extend over the entire domain of the corresponding Schrödinger equation, one chooses a lattice of localized basis functions. Some simple test calculations[170-172] show the method to be highly accurate and efficient. The method, however, needs to be tested for more realistic problems. It has been suggested[173] that the GFE technique may serve as a powerful tool for increasing further the efficiency of the

NBC methods.

In addition, Philpott[174] has also discussed a new method of treating the traditional basis states with the aim of reducing the calculational labour. The basic idea is to divide the basis functions into so-called "localized structure" functions and channel functions; the former being capable of accounting for the distortions away from the channel function which may occur within the interaction region. It appears that there may be an intrinsic connection between the division of the basis functions employed by Philpott and the one in the GFE method. Hence a detailed study on these lines may give rise to the formulation of a more sophisticated method for treating reaction problems.

Finally, Delsanto[175] and Delsanto *et al.*[176] have reported that the accuracy and efficiency of the NBC methods, especially in comparison with the eigenchannel method, can be improved drastically by introducing some modifications in the BD method. It remains to be seen, however, how these modifications compare, for example, with the energy correction to the BD method.

In conclusion, it is hoped that the NBC methods discussed so far will aid in the quest for a better understanding of the reaction processes in nuclear, atomic and molecular physics by incorporating more sophisticated and realistic models. In order to have an idea about their versatility and achievements, it is necessary to apply them to several model and realistic problems and to compare the results with the existing methods. This will be the main object in the remaining part of the thesis.

CHAPTER 4

APPLICATION TO $^{12}C(n, n)^{12}C$ REACTION

4.1 Introduction

The BD and IRM methods will be applied in the present chapter to the elastic scattering of neutrons from ^{12}C below the inelastic threshold at 4.43 MeV . In view of the typical intermediate nuclear structure phenomena observed in the corresponding excitation functions[116-120], this reaction has been the subject of several theoretical investigations from different view points[55-57,60,63,66,67,70-75,177-182].

The underlying idea in most of these works is the formation of the compound nucleus ^{13}C as a result of an s- or d- wave incident neutron interacting with the ground and/or first excited state of ^{12}C . The probable dominant configurations for some of the observed levels in ^{13}C together with the corresponding excitation energies for the low-lying levels in ^{12}C are shown schematically in figure (4.1.1). Further description of the higher energy levels of ^{13}C together with a detailed account of the corresponding positive parity states predicted by using a harmonic-oscillator and a Woods-Saxon potential are given, for example, by Robson and Van Megen[71,72].

Since the main object of the present work is to test the predictions of the BD and IRM methods, no attempt will be made to discuss the detailed spectroscopic features of the nuclei involved in the reaction under consideration. Although the ^{12}C nucleus is now considered to be collective in nature[183,186], the present calculations [Sec.4.3] will be based on the

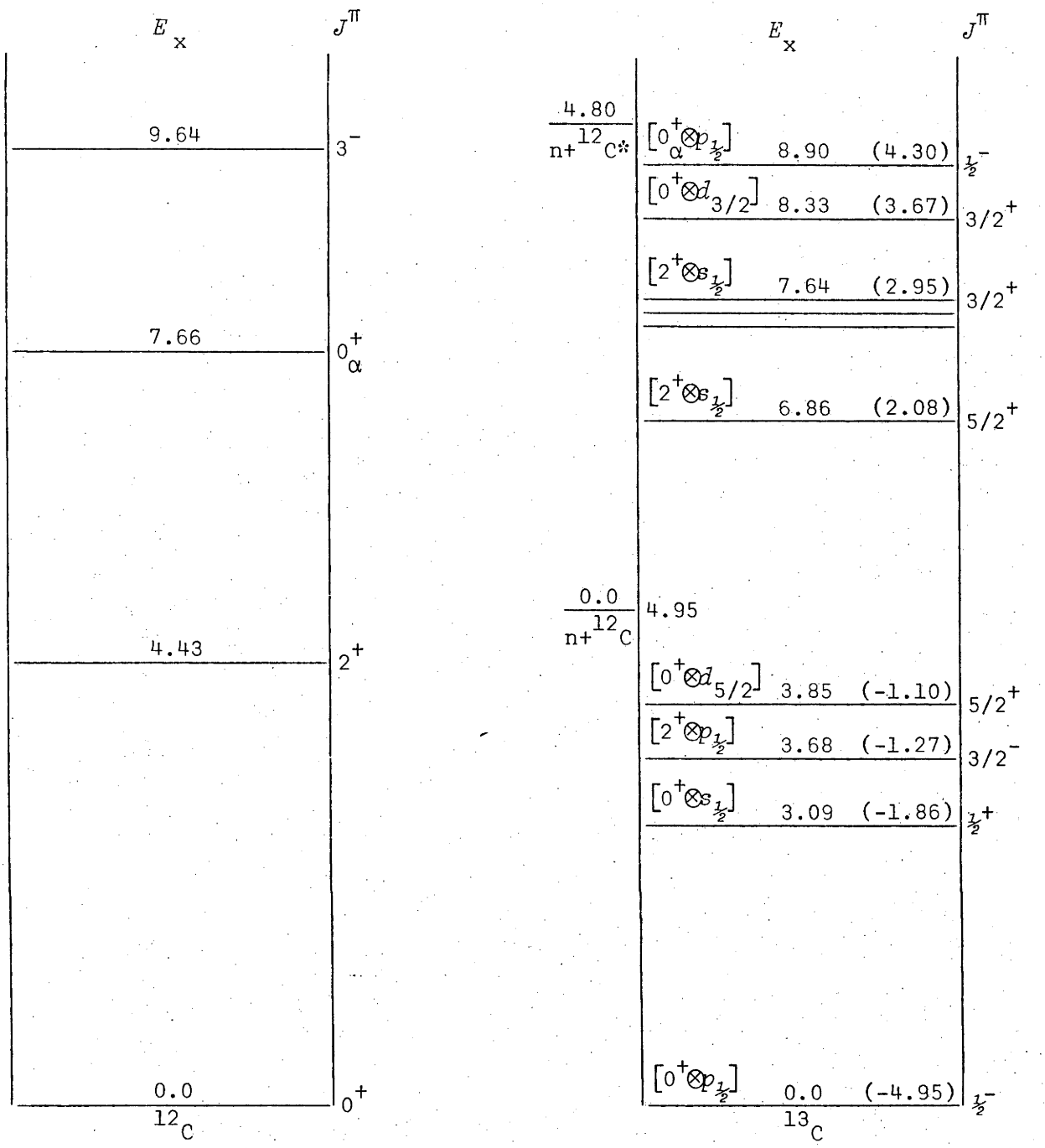

FIGURE (4.1.1): Some of the observed energy levels in ^{12}C and ^{13}C. The quantities within the parantheses are the resonance or bound state energies in the laboratory system, whereas the square brackets represent the possible dominant configurations[55,66,183-185]. Further details are given in the text and notice that the energy values are not according to scale.

weak vibrational model of Reynolds *et al.*[66] [Sec.4.2]. While this model gives a satisfactory fit to the elastic scattering cross section, it is not expected to give an adequate description of the inelastic cross section above 4.43 MeV . However, Philpott and George[75] employed the model as a test of the generalized R-matrix (GRM) method so that it is convenient to use it in the present work for comparative purposes. Moreover, for simplicity, only the positive parity states of ^{13}C will be considered.

4.2 The Nuclear Model

In the model of Reynolds *et al.*[66] an s- or d- wave neutron is assumed to move in a potential arising from the ^{12}C nucleus in its ground state or 2^+ first excited state. The basis functions describing the ^{13}C system for the internal region and satisfying the boundary conditions of eqs. (3.3.5) or (3.4.5) may be written as

$$\begin{aligned}\phi_p &= r_c^{-1}\omega_{pc}(r_c)\,|c) \\ &= r_c^{-1}\omega_{pc}(r_c)\,i^l\left[Y^{m_l}_{l\frac{1}{2}j}\otimes X_{IM}\right]^{M_J}_J , \\ &\equiv |(ljI)JM_J\rangle , \end{aligned} \tag{4.2.1}$$

where X_{IM} denote the core states, $Y^{m_l}_{l\frac{1}{2}j}$ are the usual vector-coupled spin-angle wave functions and the remaining symbols have obvious significance. The nuclear potential felt by the incident neutron is taken to be of the general Woods-Saxon form with a spin-orbit term, viz.

$$V(r) = -Vg(r) + \frac{S}{r}\frac{dg(r)}{dr}\,\sigma.l , \tag{4.2.2}$$

where

$$g(r) = \left\{1+\exp\left[\left(r-R(\hat{r})\right)/d\right]\right\}^{-1} , \tag{4.2.3}$$

with radius $R(\hat{r})$ and diffuseness d. In this model[187] the nuclear radius changes due to small harmonic vibrations of the ^{12}C nuclear surface; which is, therefore, characterized by dynamical deformation parameters $\alpha_{\lambda\mu}$, i.e.

$$R(\hat{r}) = R_0\left[1 + \sum_{\lambda\mu} \bar{\alpha}_{\lambda\mu} Y_{\lambda\mu}(\hat{r})\right] , \tag{4.2.4}$$

with

$$\bar{\alpha}_{\lambda\mu} = (-)^{\mu}\alpha_{\lambda-\mu} . \tag{4.2.5}$$

Assuming that the potential (4.2.2) depends only on the distance of the incident neutron from the nuclear surface; one can write, to first order,

$$V[r, R(\hat{r})] = V(r, R_0) - R_0 V \sum_{\lambda\mu} (-)^{\mu}\alpha_{\lambda-\mu} Y_{\lambda\mu}(\hat{r}) \frac{dg(r)}{dr} , \tag{4.2.6}$$

where, as required[66], the second term does not include any spin-orbit part and only the central part of the potential is used in calculating the derivative.

With this prescription the basis states are to be regarded as the eigenfunctions of the Hamiltonian

$$H_0 = H(^{12}C) + T_{s.p.} + V(r) , \tag{4.2.7}$$

where $H(^{12}C)$ defines the ^{12}C core states, $T_{s.p.}$ is a single particle kinetic energy operator and

$$V(r) \equiv V(r, R_0) = -Vg(r) + \frac{S}{r}\frac{dg(r)}{dr}\sigma.l . \tag{4.2.8}$$

The residual interaction coupling the single particle and core states is of the form

$$H_1 = -R_0 V \sum_{\lambda\mu} (-)^{\mu}\alpha_{\lambda-\mu} Y_{\lambda\mu}(\hat{r}) \frac{dg(r)}{dr} . \tag{4.2.9}$$

As shown in Appendix (4.2A), the matrix elements of the residual interaction are given by

$$\langle (l'j'I')JM_J|H_1|(ljI)JM_J\rangle = \sqrt{\frac{5}{4\pi}}\beta R_0 V i^{l-l'}\{\tfrac{1}{2}\hat{j}'(-)^{J+j}W(I'j'Ij|J2)$$

$$C(j'2j|-\tfrac{1}{2}0-\tfrac{1}{2})[1+(-)^{l+l'+2}]\}\int_0^\infty \omega_{p'c'}(r)\left[\frac{dg(r)}{dr}\right]\omega_{pc}(r)dr \ , \quad (4.2.10)$$

where only quadrupole vibrations are taken into consideration and $\hat{x} = (2x+1)^{\frac{1}{2}}$. In this model only matrix elements between channels involving different ^{12}C states are non-zero which implies that the results do not depend upon the sign of the deformation parameter β . The finite values of the quantities within the curly brackets are given in table (4.2.1) for total angular momenta of the system $J = \frac{1}{2}, \frac{3}{2}$ and $\frac{5}{2}$. Table (4.2.2) summarizes the vibrational model parameters as used by Reynolds *et al.* Notice that for $J^\pi = \frac{5}{2}^+$, the first excited state of ^{12}C is considered to be at 3.18 MeV .

4.3 Calculations and Results

The total elastic cross section for neutron scattering is given by

$$\sigma_{tot.el.} = \frac{2\pi}{k^2}\sum_{lj}(2j+1)|T_{lj}|^2 \ , \quad (4.3.1)$$

where the transition amplitude is related to the S-matrix [eqs. (3.3.19), (3.4.8)] as follows

$$T_{cc} = \frac{i}{2}\left(1-S_{cc}\right) \ , \quad (4.3.2)$$

where c is the incident channel with energy $E_x = \frac{\hbar^2k^2}{2\mu_c}$.

Using the model parameters of table (4.2.2) with two basis states per channel, the positive parity contributions to the total elastic cross section for total angular momenta of the system $J = \frac{1}{2}, \frac{3}{2}$ and $\frac{5}{2}$ were calculated by the BD and IRM methods with channel radii $a = 10.0$ and 7.2 fm , respectively. Most of the NBC calculations were carried out with these radii although tests indicated that both methods were independent of the

TABLE (4.2.1): Some reduced matrix elements of H_1 for the vibrational model of Reynolds *et al.*[66]. Further details are given in the text.

J^π	Configurations	$(2^+ \otimes s_{\frac{1}{2}})_J$	$(2^+ \otimes d_{3/2})_J$	$(2^+ \otimes d_{5/2})_J$
$\frac{1}{2}^+$	$(0^+ \otimes s_{\frac{1}{2}})_J$		-0.28	-0.35
$\frac{3}{2}^+$	$(0^+ \otimes d_{3/2})_J$	0.20	0.20	-0.13
$\frac{5}{2}^+$	$(0^+ \otimes d_{5/2})_J$	-0.20	0.11	0.21

TABLE (4.2.2): Vibrational model parameters

^{13}C J^{π}	first excited state ^{12}C (MeV)	deformation β	single particle potential			
			V (MeV)	S (MeV.fm^2)	R_0 (fm)	d (fm)
$\frac{1}{2}^+$, $\frac{3}{2}^+$	4.433	0.035	62.3	13.62	2.8618	0.408
$\frac{5}{2}^+$	3.180	0.080	55.1	13.60	2.8618	0.400

channel radii within the range $6.0 \leq a \leq 12.0$ fm . For the $\frac{5}{2}^+$ contributions there are four open channels above 3.18 MeV . For these cases, the iteration procedure of the IRM method was carried out using only the real part of the complex n.b.c. parameters(*) . For each method the results are the same and a comparison with the experimental cross section is shown in figure (4.3.1).

It is seen that two sharp resonances, a $\frac{5}{2}^+$ at 1.93 MeV(**) and a $\frac{3}{2}^+$ at 2.77 MeV , superimposed upon a broad $\frac{3}{2}^+$ peak and a mainly s-wave background are predicted. The NBC results are in good agreement with the observations except near the $\frac{1}{2}^-$ resonance at 3.95 MeV and the sharp peak at 2.6 MeV which are not predicted by the present model. This means that the results are also in substantial agreement with the coupled-channels calculations of Reynolds *et al.*[66] and the GRM prediction of Philpott and George[75].

Figure (4.3.2) shows a comparison between the GRM calculation of ref.[75] with eight harmonic oscillator (h.o.) basis states per channel and the NBC methods with only one basis function per channel for the $J^\pi = \frac{1}{2}^+$ and $\frac{3}{2}^+$ contributions to the total elastic cross section. The channel radii in the GRM calculation are 7.0 fm . The reason for the small discrepencies ($\sim$ 50 keV) in the positions of the resonances is not understood but may be explained by differences in the fundamental constants. The computer codes for the BD and IRM methods were written completely independently and give the same results.

Figure (4.3.3) shows standard R-matrix (SRM) calculations employing two and four basis functions per channel with $b_c = b = 0$ in all channels

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(*) At this stage the extension of the IRM method to more than one channel was not developed. However, this problem did not exist for the BD method and the results of the two methods agreed very well.

(**) All energies are in the c.m. system with origin at the ^{12}C+n separation energy.

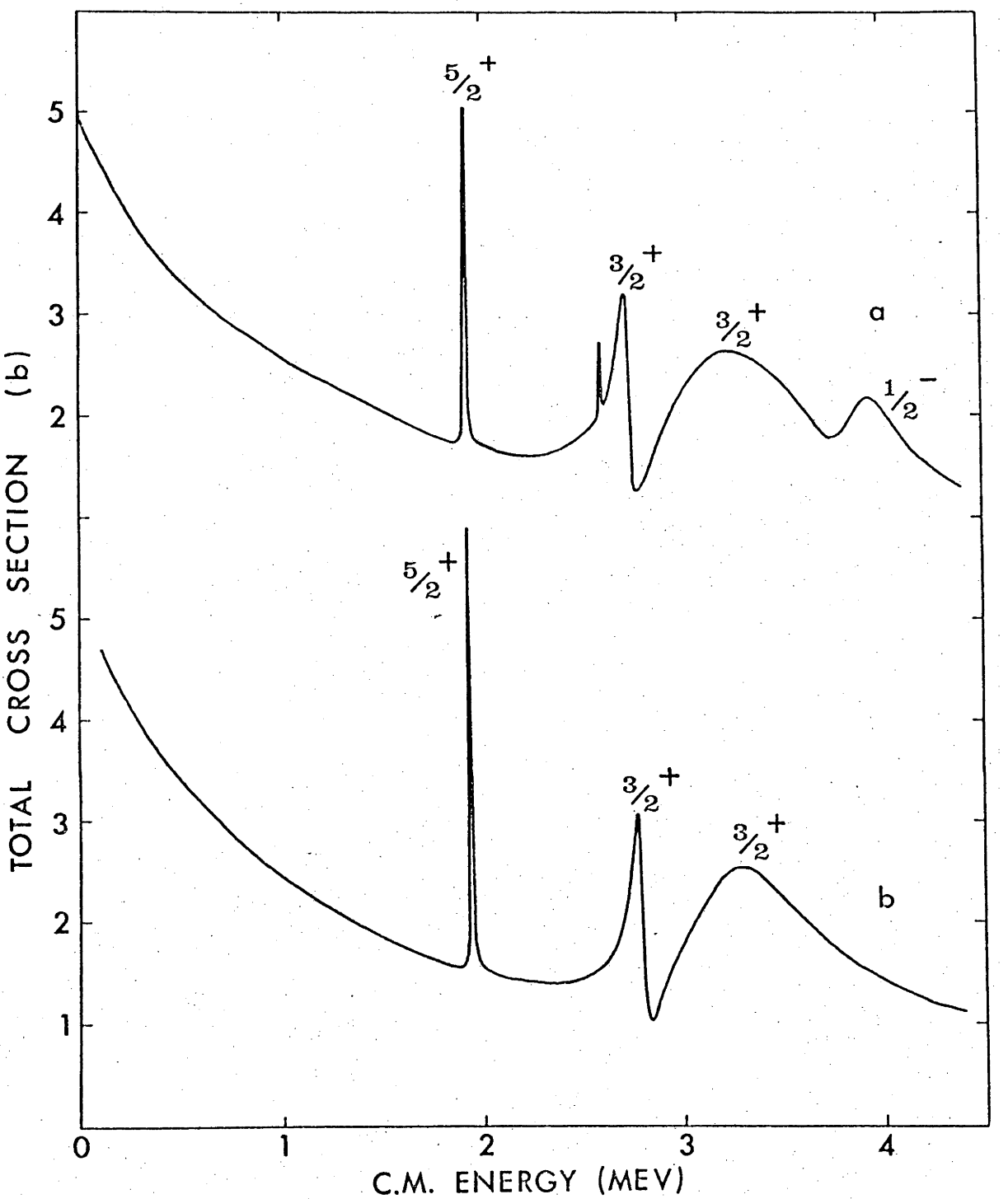

FIGURE (4.3.1): Total elastic neutron cross section of ^{12}C . The curves are (a) experiment (b) sum of the $J^{\pi} = \frac{1}{2}^+, \frac{3}{2}^+$ and $\frac{5}{2}^+$ contributions calculated by the BD and IRM methods with two basis states per channel and a = 10.0 fm and 7.2 fm respectively for the model parameters of table (4.2.2).

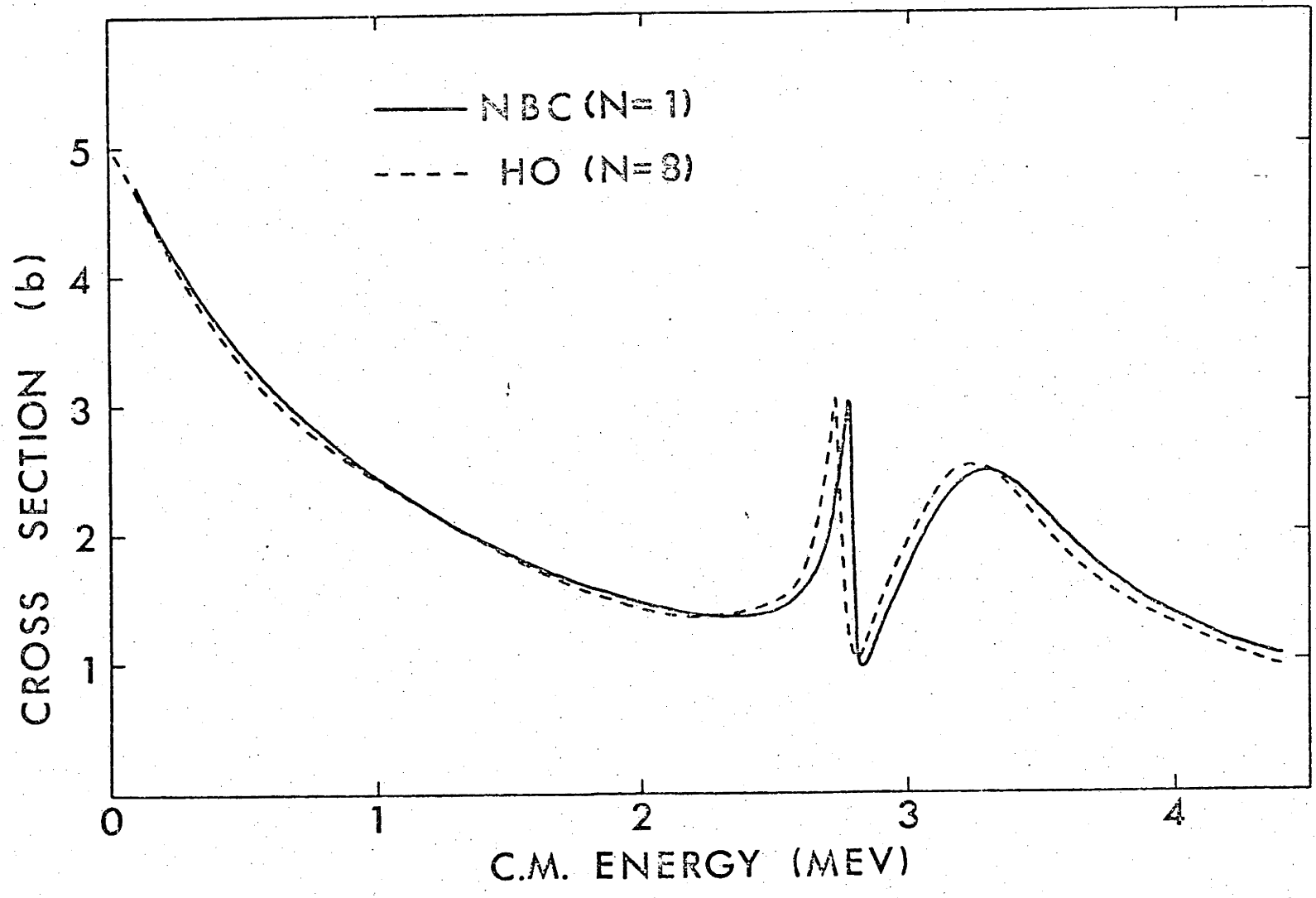

FIGURE (4.3.2): Sum of $J^{\pi} = \frac{1}{2}^{+}$ and $\frac{3}{2}^{+}$ contributions to the total elastic neutron cross section of ^{12}C, calculated by the NBC methods with one basis state per channel, compared with the GRM result of ref.[75] with eight harmonic-oscillator states per channel for the model parameters of table (4.2.2).

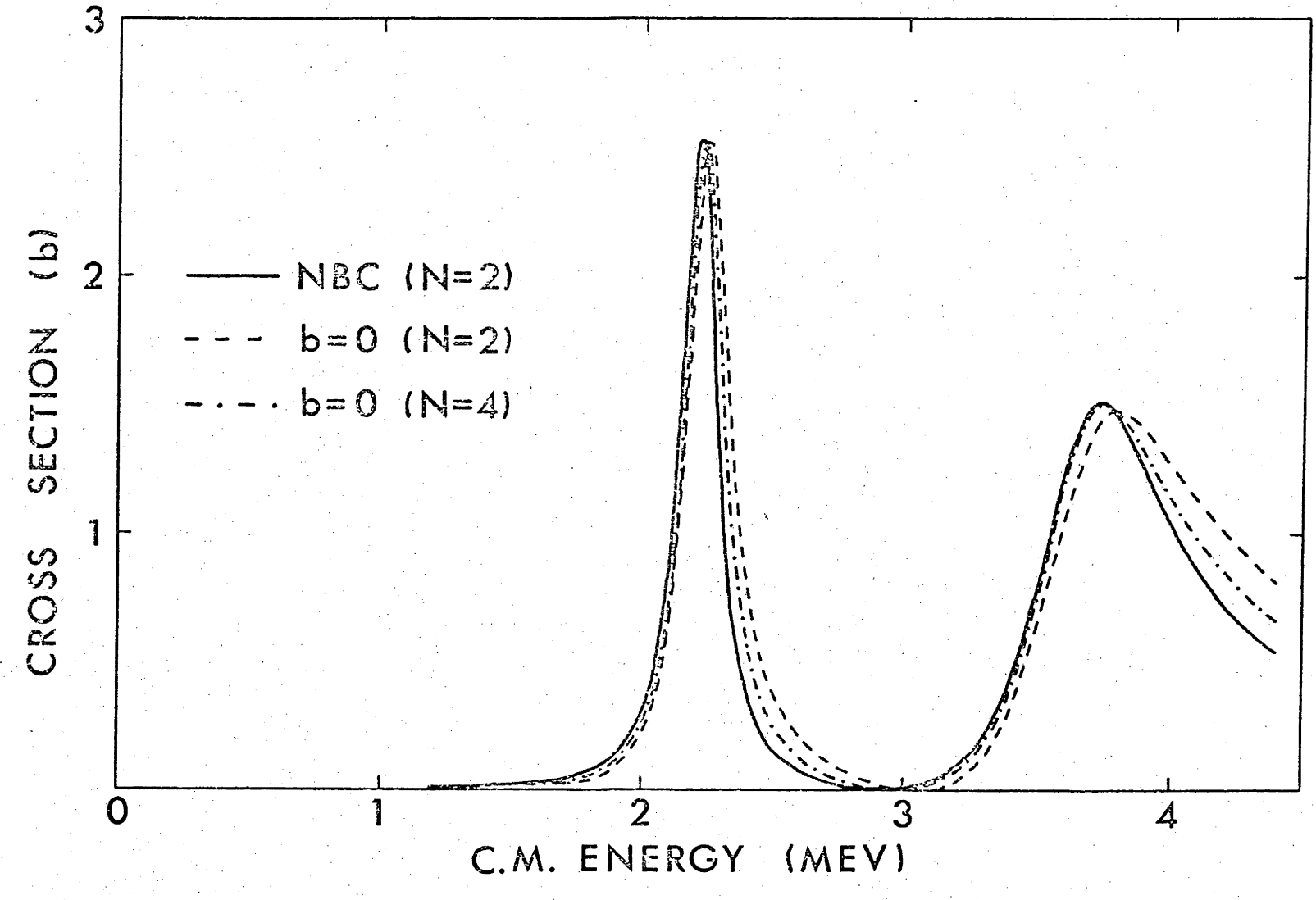

FIGURE (4.3.3): Calculated $J^{\pi} = \frac{3}{2}^{+}$ contribution to total elastic neutron cross section of ^{12}C using the SRM method for $b_c = \bar{b} = 0$ in all channels with two or four basis states per channel, compared with the NBC methods with two basis states per channel for the model parameters of table (4.2.2) and a deformation parameter $\beta = 0.168$.

for the $J^{\pi} = \frac{3}{2}^{+}$ contribution to the total elastic cross section in the case of a rather large deformation parameter $\beta = 0.168$ and channel radii $a = 7.2$ fm . This larger value of β is considered to be a more stringent test of the methods. It is seen that the SRM method converges relatively slowly for c.m. energies near 2.4 and 4.1 MeV where the n.b.c. parameters for the open channel changes in value from $-\infty$ to $+\infty$. The full curve is the converged result given by the NBC methods using two basis states per channel.

In the BD method the number of iterations required for convergence depends upon the strength of the residual interaction but in general no more than four iterations were needed in the present work. In the IRM method the required number of iterations is generally small (1 or 2) but may be quite large ($\gtrsim 10$) when the n.b.c. parameter for the open channel has a large magnitude (say $|b_c| > 100$) . In such cases the IRM method requires a minor modification since the iteration procedure often converges to a value of $|b_c| \to \infty$ and not to the n.b.c. value. This problem, which appears to arise partly from numerical difficulties associated with the small R-matrix elements for such b_c , was overcome by continuing the iteration with a b_c of smaller value and of opposite sign. Thus if from eq. (3.3.12) the value of b_c was derived to be -300 , this value was changed to +5 before the method was continued; if this still did not lead to convergence corresponding to the n.b.c. value, values of $b_c = 10, 15$, etc. were tried until convergence was achieved. This problem which tends to arise for fairly large positive values of the n.b.c. parameters, does not occur in the BD method.

4.4 Discussion and Conclusion

The two methods of the present work which employ "natural boundary condition" parameters have been found to give good agreement with the coupled-channels calculations of Reynolds *et al.*[66]. In the present methods only one or two basis functions per channel are required in contrast to the six or more harmonic oscillator basis states needed in the GRM work of Philpott and George[75]. Such a reduction in the number of basis states is very important for problems in which the number of channels is large. The BD and IRM methods discussed here converge very rapidly as the number of basis states is increased and there is no reason to suspect that either method is only semiconvergent.

In the present case the calculation of the energy-dependent basis states requires most of the computing time so that the overall efficiency of each method is very much determined by this part of the computer code. For the present problem, the two methods were found to require comparable computer time.

The main advantage of the NBC methods over SRM calculations with energy-independent basis wave functions is their rapid convergence as the number of basis states is increased. In general both treatments require few iterations to achieve a satisfactory result. In the IRM method the number of iterations may often be reduced either by applying the correction of Buttle for distant levels[63] or by using the n.b.c. parameter previously obtained at an adjacent energy as the initial value of b_c to obtain a better *initial* estimate for the S-matrix element corresponding to the incident channel.

In view of the present success of the NBC methods in describing the scattering and reaction cross sections for the case of one open channel, it may be worthwhile to apply the methods to similar realistic problems such as

α-α scattering and the $^{16}O(n, n)^{16}O$ reaction which have been treated by different *R*-matrix type methods[69,75,151]. Moreover, it is also necessary to check the reliability of the methods in the more important inelastic region.

CHAPTER 5

APPLICATION TO AN ANALYTICALLY SOLUBLE MODEL

5.1 Introduction

In order to compare the relative convergence of the various methods, it is necessary to apply them to a model for which the exact solution is known or can be calculated. For this reason, the weak vibrational model of Reynolds *et al.*[66] for which a coupled-channels calculation had already been made, was used in the last chapter to investigate the convergence of the SRM and GRM methods relative to the BD and IRM methods. However, this work was essentially restricted to the calculation of the elastic scattering cross section below the inelastic threshold.

To check the reliability of the methods in the important inelastic region, the present chapter is devoted to the application of the various methods to a model comprising two square well potentials coupled by a square well interaction. This coupled-channels problem is exactly soluble and has been used previously by other workers[35,36,47,121,167,188-191] as a test of reaction theories. It is therefore very convenient for comparative purposes.

Starting from a description of the model in the following section, the convergence (i.e. the number of basis states required) of the NBC methods which has been investigated for weak, intermediate and strong coupling interactions is discussed in Section 5.3. Therein the results are compared where possible with those of the SRM, GRM, BCRM and other related methods. Finally a summary of the main conclusions is given in Section 5.4.

5.2 Analytically Soluble Model

The model to be considered here is an s-wave (uncharged) projectile interacting with a two-state target via square well potentials. The system

is described by the Schrödinger equation

$$(H-E_x)\psi = 0 \ , \tag{5.2.1}$$

which in matrix notation may be written

$$\begin{pmatrix} T+V_{11}(r)-E_x & V_{12}(r) \\ V_{12}(r) & T+V_{22}(r)-E_x+Q \end{pmatrix} \begin{pmatrix} \psi^{(1)} \\ \psi^{(2)} \end{pmatrix} = 0 \ , \tag{5.2.2}$$

where T is the kinetic energy operator, Q is the reaction threshold energy in the second channel and the potential $V_{ij}(r)$ are of the form:

$$\left.\begin{aligned} V_{ij}(r) &= -V_{ij} \quad \text{for} \quad r \le R \\ &= 0 \qquad\qquad\ \ r > R \end{aligned}\right\} \ . \tag{5.2.3}$$

The basic coupled radial equations for the model are

$$\frac{d^2u_1(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E_x-V_{11}(r)\right]u_1(r) = \frac{2m}{\hbar^2}V_{12}(r)u_2(r) \ , \tag{5.2.4a}$$

$$\frac{d^2u_2(r)}{dr^2} + \frac{2m}{\hbar^2}\left[E_x-Q-V_{22}(r)\right]u_2(r) = \frac{2m}{\hbar^2}V_{12}(r)u_1(r) \ , \tag{5.2.4b}$$

where m is the reduced mass of the scattered particle. As shown in Appendix (5.2A), these equations can be solved exactly to obtain the radial wave functions $u_1(r)$ and $u_2(r)$ for channels 1 and 2, respectively. From these solutions, the S-matrix and associated elastic scattering and reaction cross sections can be calculated by means of the relations:

$$\sigma_{el} = \frac{\pi}{k_1^2}\left|1-S_{11}\right|^2 \ , \tag{5.2.5}$$

$$\left.\begin{aligned} \sigma_r &= \frac{\pi}{k_1^2}\left|S_{21}\right|^2 \quad \text{for} \quad E_x > Q \\ &= 0 \qquad\qquad\ \ E_x < Q \end{aligned}\right\} \ , \tag{5.2.6}$$

where S_{11} and S_{21} are the usual S-matrix elements and $k_1^2 = 2m\,E_x/\hbar^2$.

5.3 Calculations and Results

The BD and IRM methods were compared with several other methods by incorporating the analytically soluble model into the procedures described in detail in Chapters 2 and 3. As discussed in Appendix (5.3A), one of the advantages of this model is that the basis states ϕ_j - defined in eqs. (3.3.4) and (3.4.4) for both the NBC methods - can be evaluated analytically, leading to a saving of computing time.

Table (5.3.1) summarizes the different parameters of the model which were varied to simulate cases of weak, intermediate and strong coupling. A detailed description of these calculations is given in the following paragraphs.

5.3.1 INTERMEDIATE COUPLING

Several calculations have been made using the above model with the parameters of table (5.3.1) col. (a) [referred to here as intermediate coupling]. Haglund and Robson[47] have performed a SRM calculation while Purcell[121] and Garside and Tobocman[189] have used so-called generalized or extended R-matrix methods employing non-orthogonal basis states. For channel radii of 6.0 fm , Purcell required at least six harmonic oscillator states per channel to reproduce the exact results. Garside and Tobocman obtained the same result for basis states orthogonal over a hypersphere of radius 8.0 fm and hence non-orthogonal over the interior region with boundaries at 6.0 fm . In these calculations, the channel radii were chosen equal to the nuclear radii (6.0 fm) . However, this is a rather special choice since in general one cannot take the matching radii equal to the nuclear radius (e.g. a Woods-Saxon potential). Thus in the present calculations, each channel radius was taken to be 7.5 fm . This larger value also provides a more stringent test of the various methods.

TABLE (5.3.1)

Model parameters

Model Parameters	(a) Intermediate Coupling	(b) Strong Coupling	(c) Weak Coupling
V_{11} (MeV)	32.161	32.161	31.000
V_{22} (MeV)	39.022	39.022	41.000
V_{12} (MeV)	1.072	20.000	0.100
R (fm)	6.000	6.000	6.000
Q (MeV)	3.500	3.500	6.000

The results for the elastic and inelastic scattering cross sections are given in table (5.3.2) and figure (5.3.1) respectively. In each method the fixed boundary condition parameters were taken equal to zero and the lowest four levels per channel were employed. It is seen that both the NBC and BCRM methods give a good description of the cross sections while the SRM calculations are quite poor showing slow convergence in the method. The BD method including eight additional higher basis states per channel in the energy correction gives considerably improved results which are shown in the last column of table (5.3.2) and are indistinguishable from the exact results in figure (5.3.1). No results for the GRM methods with channel radii 7.5 fm are available for the model being considered. However, the calculations of Philpott and George[75] for the weak vibrational model of Reynolds *et al.*[66] indicate that $\gtrsim 10$ levels per channel would be required. For channel radii of 8.0 fm, Garside and Tobocman found that more than 20 levels per channel were needed for convergence in a SRM calculation.

The convergence of any R-matrix type reaction theory is clearly sensitive not only to the values of the matching radii but also to the strength of the channel coupling interaction. In the next subsection the effect of a substantial increase in this coupling is studied.

5.3.2 STRONG COUPLING

In this case the same model parameters were used as for the previous intermediate coupling example except that the channel coupling interaction was increased from 1.072 MeV to 20 MeV [see table (5.3.1)]. As may be expected, the convergence of all methods was considerably worse in this strong coupling case. The results obtained with the lowest six levels per channel for the elastic and inelastic cross sections are shown in figures (5.3.2) and (5.3.3), respectively. It is seen that the NBC methods give substantially better agreement with the exact calculations than either the

TABLE (5.3.2)

Elastic scattering cross sections (b) for intermediate coupling

E_x (MeV)	Exact	SRM	BCRM	NBC	BD+ Correction
0.2	1.86925	2.30209	1.87182	1.87030	1.86950
0.6	1.48436	1.74191	1.48703	1.48513	1.48422
1.0	1.13614	1.28233	1.13971	1.13705	1.13614
1.4	0.75426	0.85081	0.76032	0.75541	0.75428
1.8	0.11360	0.28496	0.12319	0.11504	0.11360
2.2	1.09383	0.68616	1.09021	1.09308	1.09374
2.6	0.98261	1.00062	0.98226	0.98283	0.98262
3.0	0.78805	0.79196	0.78743	0.78833	0.78803
3.4	0.64854	0.65780	0.64810	0.64883	0.64853
3.8	0.52466	0.55407	0.52507	0.52516	0.52461
4.2	0.46270	0.50722	0.46307	0.46323	0.46264
4.6	0.42098	0.47667	0.42121	0.42147	0.42093
5.0	0.39156	0.45397	0.39165	0.39199	0.39152
5.4	0.37038	0.43512	0.37036	0.37074	0.37034
5.8	0.35477	0.41792	0.35467	0.35506	0.35474
6.2	0.34284	0.40112	0.34268	0.34308	0.34282
6.6	0.33323	0.38407	0.33304	0.33341	0.33321
7.0	0.32495	0.36648	0.32473	0.32509	0.32494

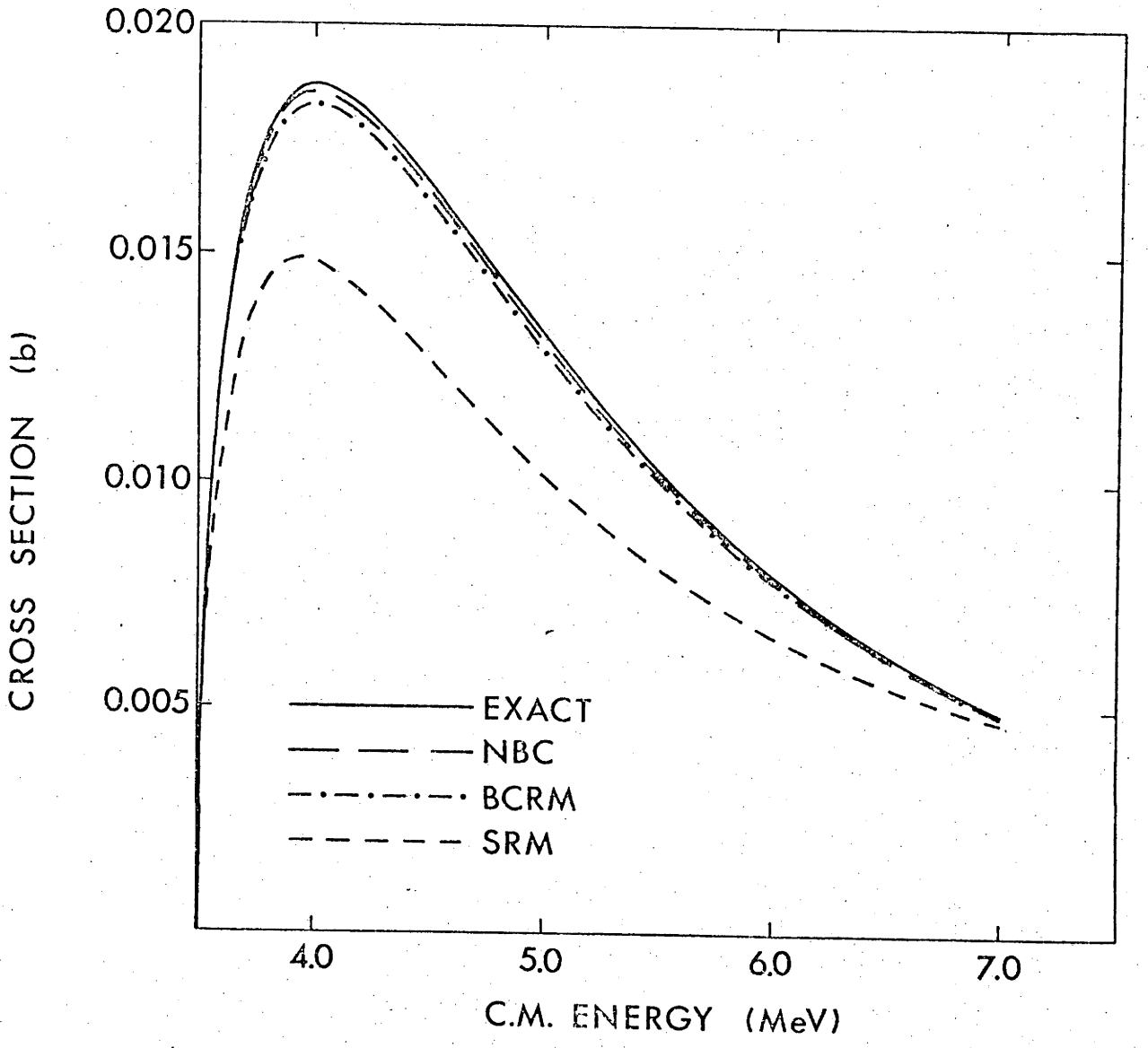

FIGURE (5.3.1): Total inelastic cross section for coupled square well model calculated by several methods for the parameters of table (5.3.1), col. (a). Each method employed $b_c = 0$ for the fixed boundary condition parameters, channel radii of 7.5 fm and the lowest four basis states per channel. The result for the BD method including the energy correction with eight additional higher basis states per channel is indistinguishable from the exact calculation.

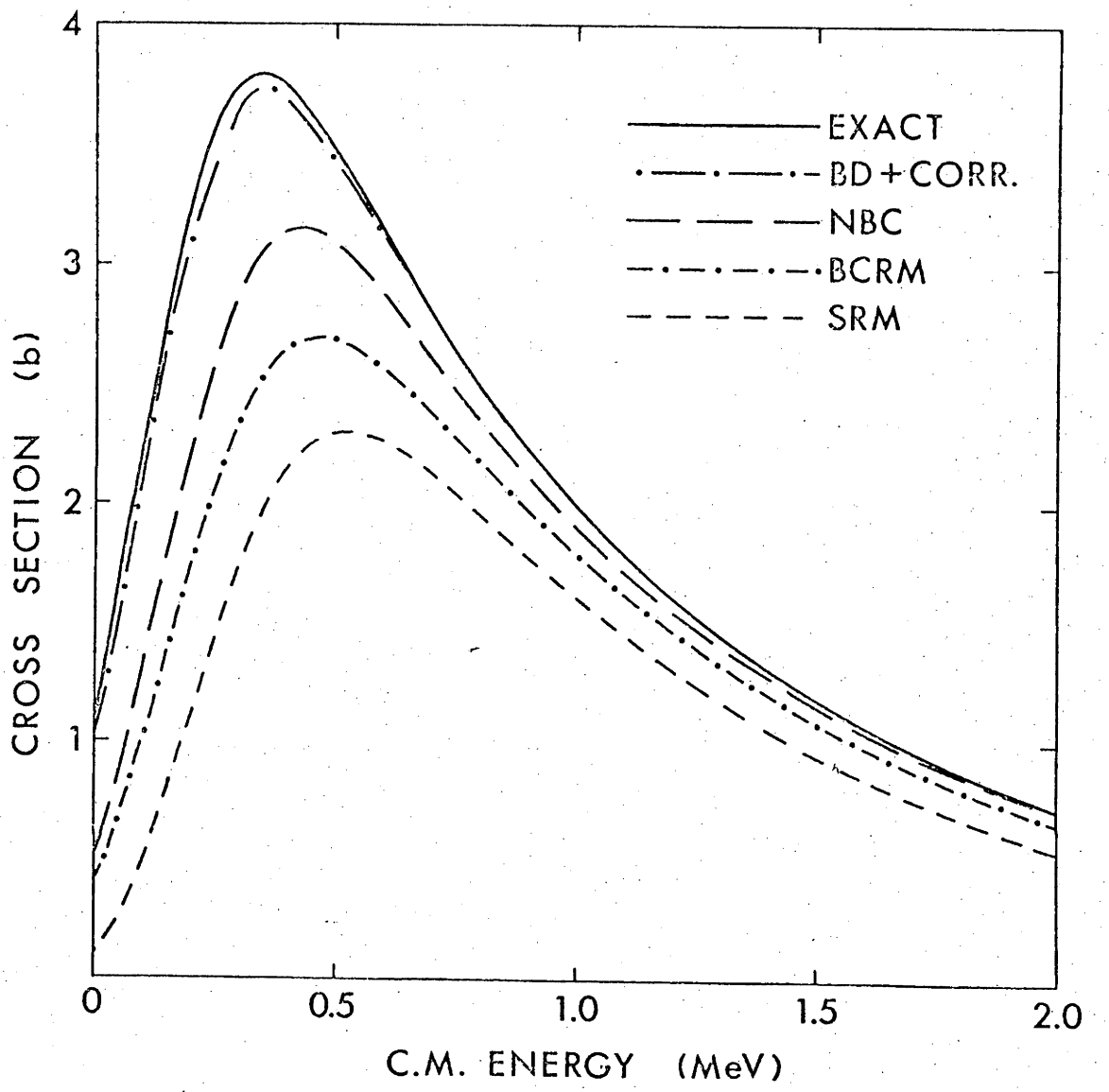

FIGURE (5.3.2): Total elastic scattering cross section for coupled square well model calculated by several methods for parameters of table (5.3.1), col. (b). Each method employed $b_c = 0$ for the fixed boundary condition parameters, channel radii of 7.5 fm and the lowest six basis states per channel. The energy correction to BD method used six additional higher basis states per channel.

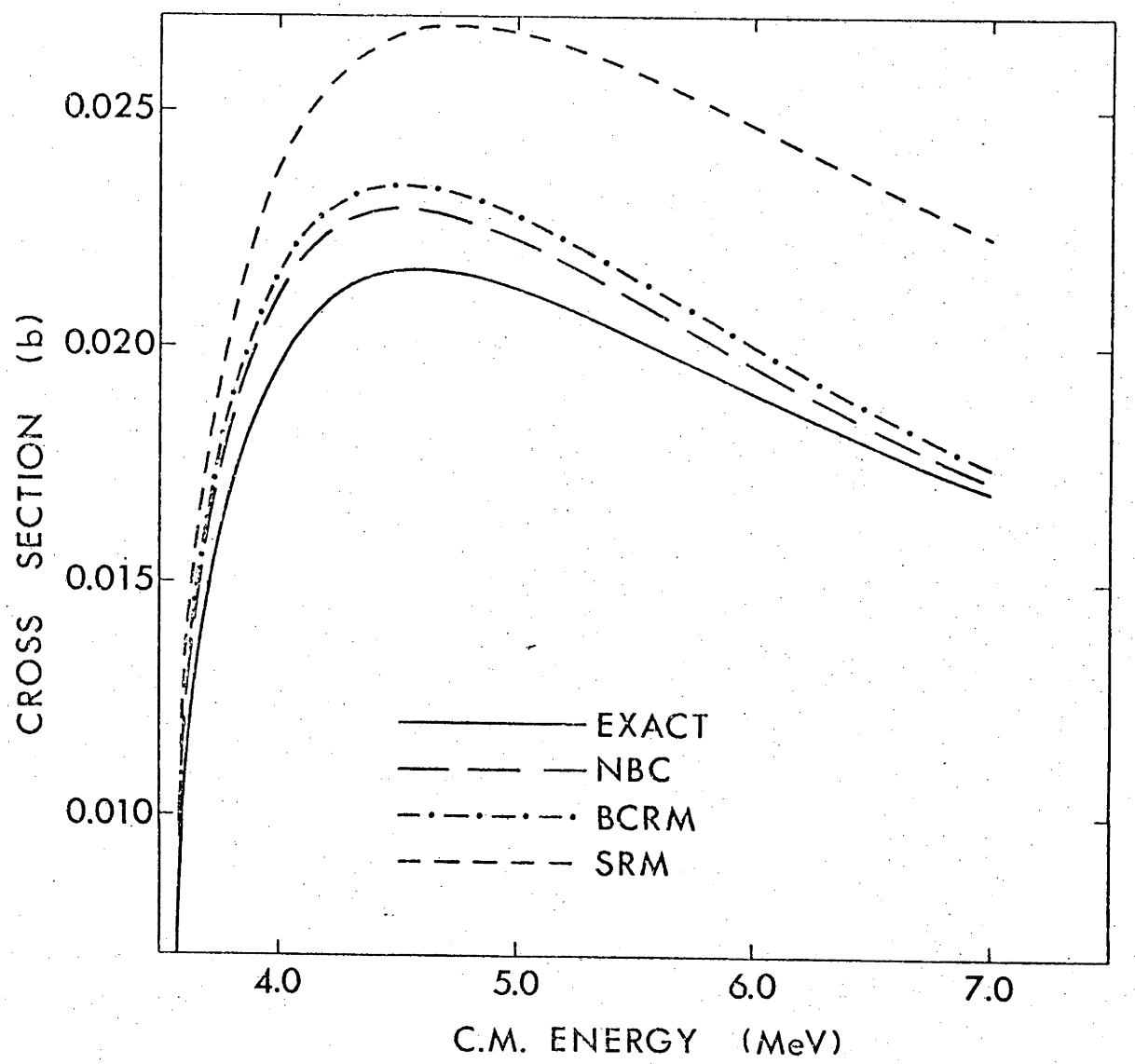

FIGURE (5.3.3): Total inelastic scattering cross section for coupled square well model calculated by several methods for the parameters of table (5.3.1), col. (b). See caption of fig. (5.3.2) for explanation of curves. The result for the BD method including the energy correction is indistinguishable from the exact calculation.

SRM method or the BCRM method. Furthermore, employing six higher levels per channel in the energy correction to the BD method as described in Section 3.5 leads to considerably improved results with little increase in the computation time. In figure (5.3.2) the energy-corrected BD method calculations are indistinguishable from the exact solution.

5.3.3 WEAK COUPLING

Lejeune and Mahaux[167] have studied the same model for the case of weak coupling [parameters of table (5.3.1), col. (c)] in the vicinity of a narrow resonance corresponding to a bound state in channel 2 embedded in the continuum. They investigated the accuracy of the one- and two-level R-matrix approximation and found that the one-level approximation plus a constant background is in general quite accurate provided that essentially n.b.c. parameters and large interaction radii are employed for the closed channel. However, for some values of the boundary condition parameter for the open channel, it was necessary to use a two-level approximation. The latter approximation corresponds closely to the case of one level per channel in the calculable methods (as distinct from the phenomenological approach of the original R-matrix theory).

Figure (5.3.4) shows a SRM calculation (curve SRM_1) using only the basis state in each channel closest to the energy of interest ($\sim$ 3.05 MeV) for boundary condition parameters $b_c = 0$ and channel radii of 6.0 fm. It is seen that the result is similar to the exact calculation except that the resonance dip is near 3.122 MeV rather than at 3.048 MeV. The curve SRM_2 shows the result of a similar calculation with n.b.c. parameters for the closed channel 2. The use of n.b.c. values for the open channel as well (i.e. NBC methods) gives a result indistinguishable from the exact curve. Thus the NBC methods, which avoid the difficulties inherent in the one-level plus background R-matrix approximation, with one level per

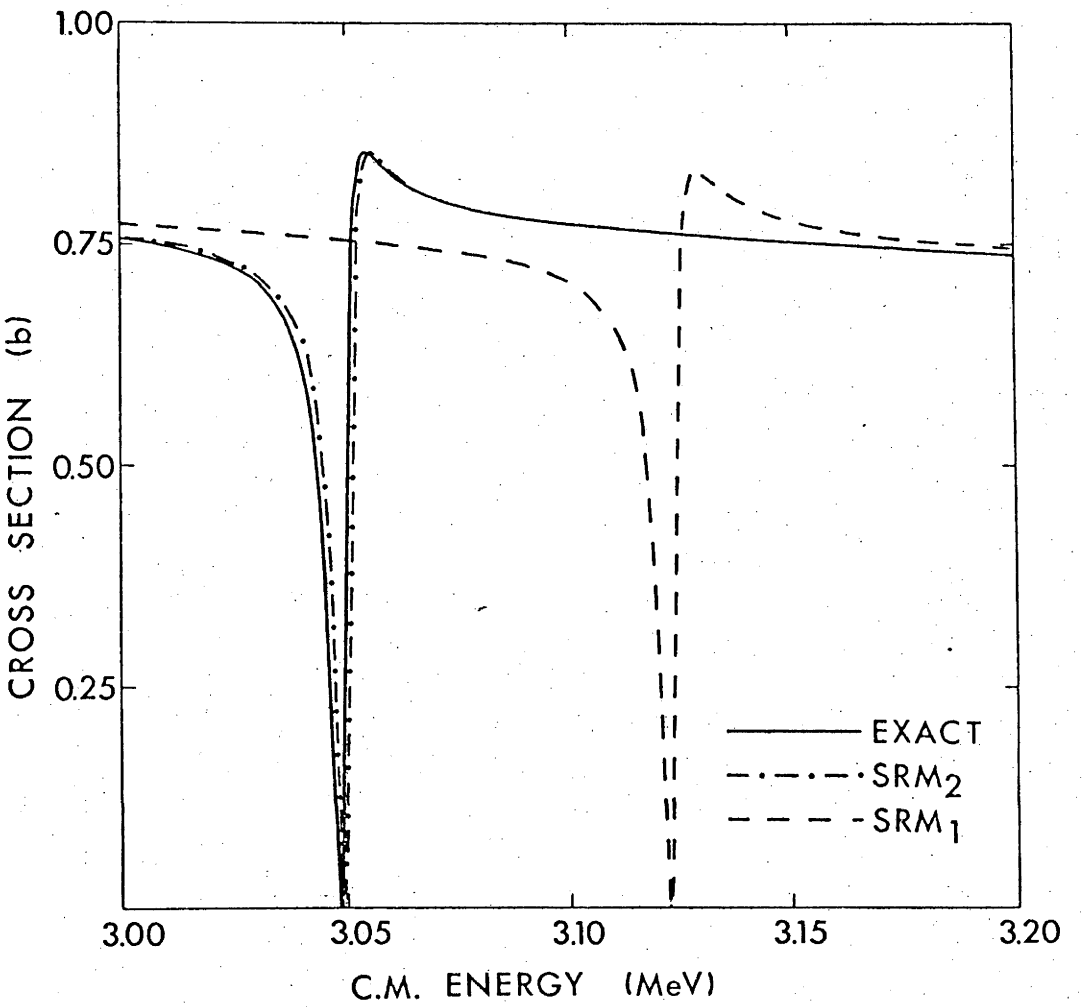

FIGURE (5.3.4): Total elastic scattering cross section for coupled square well model calculated by several methods for the parameters of table (5.3.1), col. (c). Each method employed channel radii of 6.0 fm and only the basis state in each channel closest to 3.05 MeV . Curves SRM_1 and SRM_2 are SRM calculations with $b_1 = b_2 = 0$ and with $b_1 = 0$ and n.b.c. parameters in closed channel 2 , respectively.

channel lead to results at least as accurate as two-level R-matrix approximation in a manner which can be applied to more sophisticated and realistic problems.

Lejeune and Nagarajan[35,188] have investigated the same weak coupling model using the Kapur-Peierls dispersion theory. In order to obtain a satisfactory unitarized S-matrix, it was found necessary to employ essentially a two-level approximation which is roughly equivalent to the one level per channel versions of the NBC methods. The Kapur-Peierls theory does not appear to offer any significant advantage over the NBC methods and suffers from the disadvantage of complex boundary condition parameters.

Before concluding this section, it may be worth remarking that very recently Philpott has used a similar model[191] as a preliminary test of his method proposed in ref.[174]. Unfortunately his criteria for the choice of weak and strong coupling interactions differ completely from that involved in the present work. It is therefore suggested that as a further test of the NBC methods; equivalent NBC calculations should be compared with his results. This will definitely be of value in order to understand the underlying mechanism of the various methods.

5.4 Discussion and Conclusion

In this chapter, the relative convergence of several related methods for calculating reaction cross sections from an *a priori* physical model has been compared. This problem has been the subject of recent theoretical study[92] and some of the methods discussed have had considerable application in the fields of nuclear, atomic and molecular physics.

The main purpose of the present studies was the study of NBC methods which involve an iteration procedure such that the boundary conditions applied to the basis states are varied systematically until convergence to

an optimum set of 'natural boundary conditions' is obtained. The S-matrix and associated cross sections are calculated using the n.b.c. parameters and it has been seen in Section 5.3 that in general fewer levels per channel are needed to reproduce the exact solution than are required for the SRM, BCRM and GRM methods.

The first of the NBC methods to receive wide application for the calculation of the reaction cross sections was the eigenchannel method. However, this method is extremely wasteful numerically, involving many diagonalizations of large matrices. The BD method was developed in order to eliminate these numerical deficiencies and drastically reduces the computing time involved. The IRM method, on the other hand, depends explicitly upon the n.b.c. parameters providing the best rate of convergence. Both the BD and IRM methods converge to identical results. The energy correction for neglected basis states to the BD method improves the accuracy of the method without a substantial increase in either computing time or computer storage.

The basic philosophy in all of the NBC methods is that, for the treatment of realistic problems, it is more economical in terms of computer time and storage to select the optimum set of the boundary condition parameters; thus improving the convergence of the method and reducing the dimensions of the matrices to be computed. In order for this concept to be correct, the section of the computer program which calculates the eigenvalues and wave functions of the basis set for some given boundary condition parameter must be highly efficient. Thus in the computer program, one can arrange for a preliminary routine to solve the single-particle Schrödinger equations systematically for varying values of the boundary condition parameters and to store the resultant eigenvalues. The eigenvalues associated with some arbitrary boundary condition value can then be obtained by a Lagrangian interpolation procedure from the stored values. This method has proved to be both fast and reliable, and for large scale problems relatively little computing time is required in this section of the program.

The results of the several methods have been compared in Section 5.3 for weak, intermediate and strong coupling cases for an exactly soluble model comprising two square well potentials coupled by a square well interaction. The convergence of the SRM method is generally poor and of the methods employing energy-independent basis states, the BCRM approach seems to be the most reliable; its accuracy decreasing as the coupling is increased. The BCRM method has been used extensively by Burke and co-workers[154,155] in atomic physics and has been applied in the field of molecular physics by Heller[157] and others[92]. As stated earlier, the NBC methods are automatically Buttle corrected.

The conclusion to be drawn from the present work is that for the practical calculation of reaction cross sections from a basic physical model, the NBC methods (in particular the energy corrected BD method) seem to offer the most tractable approach. This conclusion is emphasized in problems involving strong channel coupling.

CHAPTER 6

APPLICATION TO $^{12}C(p, p)^{12}C$ REACTION

6.1 Introduction

The two NBC methods discussed in Chapter 3 have been applied so far to the $^{12}C(n, n)^{12}C$ reaction and the analytically soluble coupled square well problem. Whereas the former application has shown the superiority of these methods in the case of only one open channel (essentially below the inelastic threshold), the latter example has revealed that NBC methods offer the most tractable approach for the practical calculation of reaction cross sections.

The calculations of the NBC methods for the exactly soluble model, however, involved the scattering of an uncharged s-wave (spinless) projectile interacting with a two-state target. Moreover, there were only two open channels (each of them incorporating a square well potential) above the inelastic threshold which were coupled through a square well interaction. Therefore, it may be worthwhile to test further the convergence of the NBC methods in more complicated and realistic cases involving, for example, many open channels, more sophisticated nuclear models and the effect of the Coulomb interaction. In this context, the object of the present chapter is to apply one of the NBC methods, i.e. the IRM method, in a study of the $^{12}C(p, p)^{12}C$ reaction using a macroscopic collective model very similar to that of Mikoshiba *et al*[70]. For simplicity, only the scattering of s- and d-wave protons with the ground (0^+) and the first excited state (2^+) of ^{12}C will be considered for incident energies, E_p, up to 8 MeV, without taking any explicit account of the negative parity states in the corresponding compound nucleus.

It is expected from the charge symmetry of nuclear forces that there should be a close resemblence in the properties of the excited states of the mirror nuclei ^{13}C and ^{13}N. However, a quick glance at the energy level diagram in figures (4.1.1) and (6.1.1) and table (6.1.1) shows the advantages for theoretical studies of the $^{12}C(p, p)^{12}C$ reaction over the previously studied $^{12}C(n, n)^{12}C$ reaction. The inelastic channel involving the 2^+ state of ^{12}C in the $^{12}C+n$ system is closed with the corresponding energy region of interest and the energy spectrum is dominated by negative parity states. On the other hand, the ground state of the compound nucleus ^{13}N, which is mainly of the configuration $[\{0^+ \otimes p_{\frac{1}{2}}\}; \frac{1}{2}^-]$, is only 1.94 MeV below the $^{12}C+p$ separation energy and the total cross section depicts very clearly one $\frac{1}{2}^+$ resonance, two $\frac{5}{2}^+$ resonances and two $\frac{3}{2}^+$ resonances in the energy region below and above the inelastic threshold of ^{12}C at 4.80 MeV. The first two of these resonances have been interpreted as single particle (potential) resonances with dominant configurations $[\{0^+ \otimes s_{\frac{1}{2}}\}; \frac{1}{2}^+]$ and $[\{0^+ \otimes d_{\frac{5}{2}}\}; \frac{5}{2}^+]$ respectively, and correspond to two even-parity bound states of the $^{12}C+n$ system below the inelastic threshold [see, for example, Table (6.1.1) and figure (4.1.1)]. For each J^π, the corresponding resonances can be analysed within the framework of a coupled-channels formulation. Thus the $^{12}C+p$ system is suitable for testing the applicability of the NBC methods for a realistic case involving three and four open channels above the inelastic threshold - together with the Coulomb interaction - over a wide energy range.

In order to understand the underlying nuclear dynamics through the analyses of the structure and reaction characteristics, it is necessary to

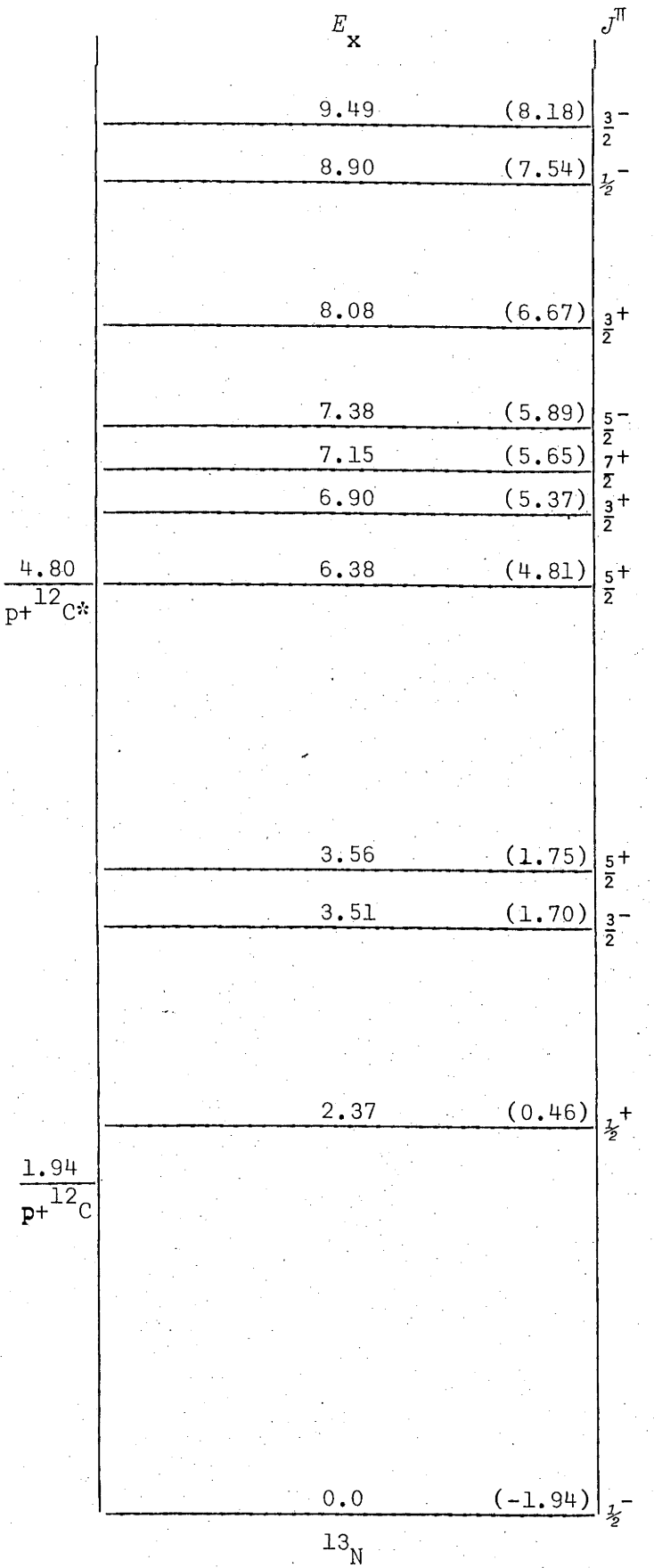

FIGURE (6.1.1): The observed energy levels in ^{13}N. The quantity within the parantheses are the resonance or bound state energies in the laboratory system. Most of the data is taken from ref.[192].

TABLE (6.1.1): Some of the observed characteristics of the low-lying positive parity states in the mirror nuclei ^{13}C and ^{13}N. The data are taken from refs[56,66,183-185,192].

J^π	E_x (MeV)		Resonance/bound state energy, $E_{c.m.}$ (MeV)		$\Gamma_{c.m.}$ (keV)		Dominant Configuration
	^{13}C	^{13}N	^{13}C	^{13}N	^{13}C	^{13}N	
$\frac{1}{2}^+$	3.09	2.37	-1.72	0.43	0	31	$[0^+ \otimes s_{\frac{1}{2}}]$
$\frac{5}{2}^+$	3.85	3.56	-1.02	1.62	0	74	$[0^+ \otimes d_{\frac{5}{2}}]$
$\frac{5}{2}^+$	6.86	6.38	1.92	4.44	6	11	$[2^+ \otimes s_{\frac{1}{2}}]$
$\frac{3}{2}^+$	7.64	6.90	2.72	4.97	124±7	115±5	$[2^+ \otimes s_{\frac{1}{2}}]$
$\frac{3}{2}^+$	8.33	8.08	3.39	6.17	1000±50	1500	$[0^+ \otimes d_{\frac{3}{2}}]$

ensure that they are generated by means of some reasonably realistic nuclear model. In fact there have been several previous attempts to study the scattering of protons from ^{12}C using different models. For example, Buttle[63] has employed a real Woods-Saxon potential and a spin-orbit term of the Thomas form within the framework of Buck's rotational model[86] in both SRM and BCRM calculations. Although the results of the BCRM method are in satisfactory agreement with the corresponding coupled-channels calculations, the nuclear model in this case is incapable of reproducing the experimental results. Van Megen[146] has also studied the same reaction within the framework of the GRM method using similar potentials in a particle-rotator model for the $^{12}C+p$ system. In this case, while the resonance energies have been predicted quite satisfactorily the phase shifts, especially in the inelastic region, are poorly described. The simplest and rather phenomenological coupled-channels calculations for analysing the upper three of the five positive parity states in ^{13}N [*cf.* table (6.1.1)] were carried out by Barnard[62] who used arbitrarily chosen finite square well potentials for the nuclear as well as the coupling interactions. On the other hand, Pascolini *et al.*[182] employed the coupled-channels formulation as described by Tamura[89] assuming a realistic optical potential for the proton-carbon interaction and the rotational model for the ^{12}C nucleus. Unfortunately, the results of the (real) phase shift analysis so obtained are quantitatively unsatisfactory; although the qualitative behaviour is fairly well reproduced for a large deformation parameter ($\beta = -0.4$) for ^{12}C.

Recently, Mikoshiba *et al.*[70] have investigated the scattering of nucleons from ^{12}C by the coupled-channels method using a realistic (macroscopic) nuclear model for the ^{12}C nucleus and giving a particular

emphasis to the resonance features in the ^{13}C and ^{13}N nuclei. Apart from a generalized Woods-Saxon and a Thomas type form factor for the central and spin-orbit interactions, respectively; they used additional terms in the potential (i.e. a spin-spin interaction, an orbital angular momentum dependent interaction and an energy dependent term) within the framework of the rotational model with a large nuclear deformation parameter. Moreover, they incorporated an empirical treatment of the negative parity levels of the compound system and did not take any account of the effect of anti-symmetrization. Except for a few minor discrepencies, the calculations based on this model seem to give a successful overall description of proton (neutron) scattering from ^{12}C for E_p (E_n) up to 8.0 (4.0) MeV in the laboratory system.

Thus it appears to be quite reasonable to incorporate the nuclear model of Mikoshiba *et al.* for carrying out the present IRM calculations. It may be worth emphasizing at this stage that the main object of the present work is to apply the IRM method to the case of several open channels for a realistic problem and compare the results with the corresponding coupled-channels and SRM calculations. For this reason, starting from a detailed development of the IRM method as applied to the $^{12}C(p, p)^{12}C$ reaction in the next section, Section 6.3 will be devoted to a thorough description of the nuclear model and the typical form factors for the nuclear, spin-orbit and Coulomb interactions. In Section 6.4 the method of calculation and the main results of the phase shift analyses will be described. Finally, an account of the main conclusions drawn from the present work together with suggestions for further developments and improvements will be given in Section 6.5.

6.2 The IRM Method Formulation

The essentials of the IRM method for a two-body system incorporating one or more open channels have been discussed in Section 3.4. In the present section, the application of the IRM method explicitly to the $^{12}C+p$ system will be discussed.

Let $\Psi(r, \zeta)$ be the complete wave function of the system; where r and ζ denote, respectively, the coordinates of the proton and the internal coordinates of the ^{12}C nucleus. The corresponding Schrödinger equation in the barycentric subspace may be written as

$$(H-E_x)\psi(r, \zeta) = 0 \ , \tag{6.2.1}$$

with the total Hamiltonian

$$H = T + H_t(\zeta) + V_0 + H_1 \tag{6.2.2}$$

where T is the kinetic energy operator for the relative motion, $H_t(\zeta)$ is the ^{12}C Hamiltonian and V_0 and H_1 stand, respectively, for the diagonal and non-diagonal parts of the proton-carbon interaction. The explicit forms of the interactions will be elaborated in the following section. The total wave function may be expanded in eigenstates of total angular momentum J such that

$$\Psi(r, \zeta) = \sum_c r_c^{-1} u_c(r_c)|c) \ , \tag{6.2.3}$$

with

$$|c) = \sum_{m_j M} C(jI_n J|m_j M M_J) Y^{m_l}_{l\frac{1}{2}j} \Phi_{I_n M}(\zeta)$$

and

$$Y^{m_l}_{l\frac{1}{2}j} = \sum_{m_l m_s} C(l\tfrac{1}{2}j|m_l m_s m_j) i^l Y^{m_l}_l(\theta, \phi)\chi_{\frac{1}{2}m_s} \ ,$$

where $\chi_{\frac{1}{2}m_s}$ is the spin wave function of the proton and $\Phi_{I_n M}(\zeta)$ is the

wave function of ^{12}C in its nth excited state, with spin I_n and Z-component M which satisfies

$$H_t(\zeta)\Phi_{I_n M}(\zeta) = \omega_n \Phi_{I_n M}(\zeta) \ , \qquad (6.2.4)$$

and the remaining symbols have obvious significance.

As usual, the configuration space is divided into an internal and an external region at $r_c = a_c$; with a_c being chosen large enough so that any polarizing interaction is within the internal region. In view of the assumptions mentioned in the previous section, only the values $J^\pi = \frac{1}{2}^+$, $\frac{3}{2}^+$ and $\frac{5}{2}^+$ will be considered in the present work. For $J^\pi = \frac{1}{2}^+$, there are three channels corresponding to the configurations $[0^+ \otimes s_{\frac{1}{2}}]$, $[2^+ \otimes d_{\frac{3}{2}}]$ and $[2^+ \otimes d_{\frac{5}{2}}]$; whereas for $J^\pi = \frac{3}{2}^+$ and $\frac{5}{2}^+$ there are four analogous channels. For each J^π , all the corresponding channels (say M in number) are open above $E_x = 4.43$ MeV and there are M degenerate solutions of the Schrödinger equation (6.2.2). In the asymptotic region $(r_c \geq a_c)$, these solutions assume the following form:

$$\Psi(r, \zeta) \equiv \psi_k = \sum_{\tilde{c}} \left[I_{\tilde{c}}\delta_{k\tilde{c}} - S_{k\tilde{c}} O_{\tilde{c}}\right] - \sum_{\bar{c}} S_{k\bar{c}} O_{\bar{c}} \ , \quad k = 1, \ldots, M \ , \qquad (6.2.5)$$

where, as in eq. (3.4.12), $\tilde{c}$ ($\bar{c}$) denotes open (closed) channels, S_{kc} are the usual S-matrix elements and the unit flux incoming $(I_{\tilde{c}})$ and outgoing $(O_{\tilde{c}})$ proton waves plus the ^{12}C nucleus are defined as follows:

$$I_{\tilde{c}} = \frac{I_{\tilde{c}}}{\sqrt{V_{\tilde{c}} r_c}} \, |\tilde{c}) = O^*_{\tilde{c}} \ , \qquad (6.2.6)$$

with $V_{\tilde{c}}$ $\left(= \frac{\hbar k_{\tilde{c}}}{\mu_{\tilde{c}}}\right)$ being the relative velocity in channel $\tilde{c}$ and the radial wave functions $I_{\tilde{c}}$ and $O_{\tilde{c}}$ are such that[18)]

$$I_{\tilde{c}} = O_{\tilde{c}}^{*} = \{G_{\tilde{c}}(\rho_{\tilde{c}}) - iF_{\tilde{c}}(\rho_{\tilde{c}})\} e^{i\omega_c} , \qquad (6.2.7)$$

for $\rho_{\tilde{c}} = k_{\tilde{c}} r_c$ and $k_{\tilde{c}} = [2\mu_{\tilde{c}}(E_x - Q_{\tilde{c}})]^{\frac{1}{2}}/\hbar$. Here E_x, μ_c and Q_c are the excitation energy, reduced mass and threshold energy in channel c ; F_c (G_c) is the regular (irregular) Coulomb function satisfying the Wronskian relation

$$W(G_c, F_c) = G_c \frac{dF_c}{d\rho_c} - \frac{dG_c}{d\rho_c} F_c = 1 , \qquad (6.2.8)$$

and the asymptotic conditions

$$F_c \sim \sin\left(\Delta_c - \frac{l\pi}{2}\right) , \quad G_c \sim \cos\left(\Delta_c - \frac{l\pi}{2}\right) . \qquad (6.2.9)$$

In the above relations

$$\Delta_c \equiv \rho_c - \eta_c \log 2\rho_c + \sigma_l ,$$

and the Coulomb field parameter (η_c) and the Coulomb phase shift (σ_l) for the system are given by

$$\eta_c = Z_p Z_c e^2/\hbar V_c , \qquad (6.2.10')$$

$$\omega_c = \sigma_l - \sigma_0 = \sum_{t=1}^{l} \tan^{-1}(\eta_c/t) , \qquad (6.2.10'')$$

with $\sigma_0 = \arg \Gamma(1+i\eta_c)$ and $Z_p e$, $Z_c e$ are the proton and ^{12}C charges and $\hbar = h/2\pi$, where h is the Plank's constant. The wave functions $O_{\bar{c}}$, on the other hand, are the closed channel analogues of $O_{\tilde{c}}$, e.g.

$$O_{\bar{c}} = \frac{W_{\bar{c}}(\rho_{\bar{c}})}{r_c} |\bar{c}) , \qquad (6.2.11)$$

with $\rho_c = k_{\bar{c}} r_c$ and $k_{\bar{c}} = [-2\mu_{\bar{c}}(E_x - Q_{\bar{c}})]^{\frac{1}{2}}/\hbar$. The quantities $W_{\bar{c}}(\rho_{\bar{c}})$ are the usual Whittaker functions[193]

$$W_c(\rho_c) = e^{-\rho_c} \rho_c^{l+1} {}_1F_1(l+1-\eta_c, 2l+2, 2\rho_c) , \qquad (6.2.12)$$

where ${}_1F_1(a, b, Z)$ represents the corresponding confluent hypergeometric function. These functions can be calculated accurately using standard methods[194].

Following the procedure discussed in Section 3.4, the Schrödinger equation (6.2.1) is to be solved by introducing the boundary condition operator $L(b_c)$ [*cf.* eq. (3.3.1)]. Expanding the total wave function ψ_k in terms of the eigenstates, ϕ_j, of the single-particle Hamiltonian H_0 $(= H - H_1)$ satisfying eq. (3.4.4) and transforming the set of wave functions ψ_k into the standing wave solutions for the open channels one obtains

$$\chi_{k'} = \sum_{\tilde{c}} \left[(T^-)_{k'\tilde{c}} I_{\tilde{c}} - (T^+)_{k'\tilde{c}} O_{\tilde{c}}\right] - \sum_{\bar{c}} (F^-)_{k'\bar{c}} O_{\bar{c}} \ , \qquad (6.2.13)$$

with

$$(T^{\pm})_{k'k} = V_{k'k} e^{\pm i\delta_{k'k}} \ , \qquad (6.2.14)$$

and $(F^-)_{k'\bar{c}}$ defined in eq. (3.4.15). This prescription enables one to formulate the set of equations (3.4.17) for the present problem which incorporates, at the most, four open channels above and one open plus three closed channels below the inelastic threshold. For the former situation some straightforward but lengthy calculations give the four sets of equations [i.e. eqs. (6.2A.1)-(6.2A.4)] summarized in Appendix (6.2A). Below the inelastic threshold, on the other hand, there is only one open channel and the corresponding set of equations is given by eq. (6.2A.5).

Once the R-matrix elements $R_{c'c''}$ [*cf.* eq. (3.4.9)] are calculated in a definite basis obtained by following the procedure described in Section 3.4, these sets of equations can be solved. Having determined the phase shift $\delta_{k'k}$, and the relative amplitudes $\overline{V}_{k'c'}$ corresponding to each open

channel, the overall formulation can be employed for evaluating the matrix elements $(T^{\pm})_{k'k}$ of eq. (6.2.14). Finally, the S-matrix is written in the form

$$S_{k\tilde{c}} = \sum_{k''} \left[(T^{-})^{-1}\right]_{kk''} [T^{+}]_{k''\tilde{c}} , \qquad (6.2.15)$$

so that the total elastic and inelastic cross sections together with other observable quantities can be calculated by using standard relations. The complex phase shifts $\lambda_c \left(= \delta_c + i\theta_c\right)$ are connected to the elements of the scattering matrix for the incident channel, c, through the relation

$$S_{cc} = e^{2i\lambda_c} = \tau_c e^{2i\delta_c} , \qquad (6.2.16)$$

where $\tau_c = e^{-2\theta_c}$. This quantity is a measure of the absorption of the corresponding partial wave in other open channels and may be referred to as the "inelasticity" or "damping" factor.

6.3 The Nuclear Model

Assuming that the low-lying states of the ^{12}C nucleus have a strong collective rotational nature, the corresponding collective motion can be described in terms of a permanent deformation of the nuclear shape. In the model of Mikoshiba *et al.*[70] the proton-carbon interaction is approximated by a generalized optical-model potential

$$V(r, \theta, \phi) = -V_c f(r) + V_{s.o.}(\sigma.l) \frac{\lambda_\pi^2}{r} \frac{d}{dr} f(r) + V_{Coul} , \qquad (6.3.1)$$

where $\frac{1}{2}\sigma$ and l are the spin and orbital angular momentum operators of the incident proton and $\lambda_\pi = \hbar/m_\pi c$ is the π-meson Compton wavelength. The form factor $f(r)$, the strengths of the central (V_c) and spin-orbit $(V_{s.o.})$ potential and the Coulomb potential V_{Coul} may depend on the

dynamical variables of the system in a complicated manner. These quantities will, therefore, be discussed separately.

(i) The form factor: The form factor $f(r)$ is assumed to be a Woods-Saxon form:

$$f(r) = [1+\exp\{(r-R)/a\}]^{-1} , \qquad (6.3.2)$$

where a is the diffuseness parameter and the polar angular dependence of the nuclear radius R for the strongly deformed (rotational) ^{12}C nucleus having an axial symmetry is such that

$$R = R_0\left[1 + \sum_\lambda \beta_\lambda Y_{\lambda 0}(\theta')\right] , \qquad (6.3.3)$$

where β_λ is the nuclear deformation parameter and the angle θ' refers to the body-fixed system. The quantity R_0 is such that $R_0 = r_0 A^{\frac{1}{3}}$ where A is the atomic number of ^{12}C and r_0 is the radius parameter. The expression (6.3.3) may be substituted into eq. (6.3.2) in order to get a power-series expansion of the potential in the form

$$f(r, \theta, \phi) = \sum_n V^{(n)}(r)\left(\sum_\lambda \varepsilon_\lambda\right)^n , \qquad (6.3.4)$$

with

$$V^{(n)}(r) = \frac{1}{n!}\left(\frac{R_0}{a}\right)^n \frac{d^n f(r)}{dr^n} , \qquad (6.3.5)$$

and

$$\varepsilon_\lambda = \beta_\lambda Y_{\lambda 0}(\theta') = \sum_\mu \beta_\lambda D^\lambda_{\mu 0}(\theta_i) Y_{\lambda\mu}(\theta, \phi) . \qquad (6.3.6)$$

Here θ_i stands for the Euler angles between the body-fixed and the space-fixed coordinates and $D^\lambda_{\mu 0}(\theta_i)$ is a rotation matrix[195]. However, the power-series expansion no longer remains an accurate approximation for those nuclei which have a large value of the deformation parameter β_λ. Therefore,

it is more convenient to expand the potential in spherical harmonics $Y_{\lambda\mu}(\theta, \phi)$, i.e.

$$f(r) = \sum_{\lambda\mu} f_\lambda(r) D^{\lambda}_{\mu 0}(\theta_i) Y_{\lambda\mu}(\theta, \phi) \ , \qquad (6.3.7)$$

where the radial form factor

$$f_\lambda(r) = 4\pi \int_0^1 \left[1+\exp\left[\left\{r-R_0\left(1 + \sum_{\lambda'} \beta_{\lambda'} Y_{\lambda' 0}(\theta')\right)\right\}/a\right]\right]^{-1} Y_{\lambda 0}(\theta') d(\cos\theta') \ , \qquad (6.3.8)$$

for each given λ is the sum of contributions from an infinite number of terms in the power-series expansion in $\sum_{\lambda'} \varepsilon_{\lambda'}$. The expansion (6.3.7) is a better approximation than the power-series expansion (6.3.4).

(ii) The potential strengths: Following Mikoshiba *et al.*, the strength of the central potential is given by

$$V_c = V_0 - a_E E_n + (\sigma.I) V_{\sigma I} + (l.l) V_{ll} \ , \qquad (6.3.9)$$

where the constants V_0, a_E, $V_{\sigma I}$ and V_{ll} , together with the other parameters for the optical potential are given in table (6.3.1) and have the same values as set 5 of ref.[70]. The energy term $(-a_E E_n)$ is used to describe the energy dependence of the central potential relative to the ^{12}C states. Notice that $E_n = E_x$ or $E_x - 4.43$ MeV , where E_x is the centre of mass energy of the incident proton, corresponds to the ground (0^+) or the first excited state (2^+) of ^{12}C . If I be the spin operator for this nucleus, the spin-spin term $[(\sigma.I) V_{\sigma I}]$ emerges from the spin dependence of the nucleon-nucleon interactions and accounts for the correction to the interaction from the 2^+ excited nucleus, arising from treating the nucleus as a whole. The importance of this interaction in realistic nuclear problems is widely discussed in the literature[86,197-199]

TABLE (6.3.1): The potential parameters for the $^{12}C(p, p)^{12}C$ reaction calculations. The values correspond to the set 5 of the coupled-channels calculations by Mikoshiba *et al.*[70]

β	a_E	a (fm)	r_0 (fm)	V_0 (MeV)	$V_{s.o.}$ (MeV)	$V_{\sigma I}$ (MeV)	V_{ll} (MeV)
-0.5	0.26	0.65	1.25	54.37	6.5	0.37	-0.44

and a correct estimation of the interaction strength $V_{\sigma I}$ is expected to depend on the details of the nucleon-nucleon interaction together with the $^{12}C^{*}(2^{+})$ wave function. However, as stressed by Mikoshiba *et al.*, this quantity may be treated as a phenomenological parameter so that the overall interaction can give a sufficiently large splitting for the $\frac{5}{2}^{+} - \frac{3}{2}^{+}$ doublet around E_p = 5 MeV in the system under consideration. Finally, the orbital angular momentum term $[(1.1)V_{ll}]$ may be interpreted as the effect of a large diffuseness of ^{12}C or of exchange between the incident proton and the ^{12}C nucleons. The importance of this term in the present model is to improve both the resonance energy of the first $\frac{5}{2}^{+}$ level and the total inelastic cross sections in $^{12}C+p$ system. The strength V_{ll} was also adjusted phenomenologically in ref.[70]. Although the strength of the spin-orbit potential (i.e. $V_{s.o.}$) may also depend on the energy, it will be assumed to be constant as in the corresponding coupled-channels calculations[70].

(iii) **The Coulomb potential:** Assuming the ^{12}C nucleus to be a sphere of radius R_{co} with uniform charge distribution, the Coulomb potential for the $^{12}C+p$ system can be written as

$$V_{Coul} \equiv V_{co}(r) = \xi f_{co}(r, R_{co}) \qquad (6.3.10)$$

where the parameter $\xi = Z_p Z_c e^2$ and the Coulomb form factor is such that

$$f_{co}(r, R_{co}) = \frac{1}{r}\,\theta(r-R_{co}) + \frac{1}{2R_{co}}\left\{3 - \left(\frac{r}{R_{co}}\right)^2\right\}\theta(R_{co}-r) \ , \qquad (6.3.11)$$

with $\theta(X) = 0$ if $X < 0$ and $\theta(X) = 1$ if $X > 0$. In view of the collective nature of the target nucleus, a more accurate treatment of the Coulomb potential should incorporate in some way the nuclear deformation in

the form factor (6.3.11). In analogy with the radial form factor $f_\lambda(r)$ in eq. (6.3.8), the present calculations will employ the following expression for the Coulomb form factors

$$f_{co}(r, R_{co}) \equiv f_{co(\lambda)}(r) = \left\{\sqrt{4\pi}\int_0^1 Y_{\lambda 0}(\theta')\left[3 - \left(\frac{r}{R_{co\lambda}}\right)^2\right](2R_{co\lambda})^{-1} d(\cos\theta')\right\}$$

$$\theta(R_{co}-r) + \frac{1}{r}\,\theta(r-R_{co}) \quad , \qquad (6.3.12)$$

with $R_{co\lambda} = R_{co}\left[1 + \sum_{\lambda'} \beta_{\lambda'} Y_{\lambda' 0}(\theta')\right]$. Alternatively, following Tamura[89], one may use a power-series expansion similar to eq. (6.3.4). However, for the Coulomb interaction, the final results are not very sensitive to the different treatments of the deformation[70].

With the above prescription the total Hamiltonian of the system can be written as

$$H = H_0 + H_1 \qquad (6.3.13)$$

where

$$H_0 = H_t(\zeta) + T + \tilde{V}_c \tilde{f}_0(r) + V_{s.o.}(\sigma.l)\,\frac{\lambda_\pi^2}{r}\frac{d\tilde{f}_0(r)}{dr} + \xi f_{co(0)}(r) \quad , \qquad (6.3.14)$$

and

$$H_1 = V_{\sigma I}(\sigma.I)\tilde{f}_0(r) +$$

$$\sum_{\lambda(\neq 0)\mu} \{\tilde{V}_c f_\lambda(r) + \sqrt{4\pi}\xi f_{co(\lambda)}(r)\} D^\lambda_{\mu 0}(\theta_i) Y_{\lambda\mu}(\theta, \phi) \quad , \qquad (6.3.15)$$

with

$$\tilde{f}_0(r) = \frac{1}{\sqrt{4\pi}} f_0(r) \quad , \qquad (6.3.16)$$

and

$$\tilde{V}_c = -\{V_0 - a_E E_n + (1.1)V_{ll}\} \quad , \qquad (6.3.17)$$

and the remaining symbols have obvious meaning.

Finally, the matrix elements of the residual interaction can be written in the following forms [Appendices (6.3A1), (6.3A2)]:

$$\langle \phi_{p'} | \bar{H}_1 | \phi_p \rangle = \Big\{ (-1)^{\frac{1}{2}+j+j'+l'+I+J} \sqrt{6I(I+1)}\hat{I}\hat{j}\hat{j}' W(\tfrac{1}{2}\tfrac{1}{2}jj'|1l') \; W(jIj'I'|Jl)\delta_{ll'}\delta_{II'}\delta_{JJ'}\delta_{M_J M_J'} \Big\} V_{\sigma I} \int_0^\infty \omega_{p'c'}(r)\tilde{f}_0(r)\omega_{pc}(r)dr \ , \quad (6.3.18)$$

and

$$\langle \phi_{p'} | \tilde{H}_1 | \phi_p \rangle = \sum_{\lambda \neq 0} \left(\frac{2\lambda+1}{4\pi} \right)^{\frac{1}{2}} i^{l-l'} \{ C(I\lambda I'|000) C(l\lambda l'|000) W(\lambda l j' \tfrac{1}{2}|l'j) \; W(\lambda j I' J|j' I) \} \int_0^\infty \omega_{p'c'}(r) \left[\tilde{V}_c f_\lambda(r) + \sqrt{4\pi}\xi f_{\mathrm{co}(\lambda)}(r) \right] \omega_{pc}(r)dr \ , \quad (6.3.19)$$

where $H_1 = \bar{H}_1 + \tilde{H}_1$ and $|\phi_p\rangle = r_c^{-1}\omega_{pc}(r_c)|c)$. The quantities within the curly brackets are given in tables (6.3.2), (6.3.3) and (6.3.4) for the required values of J^π .

6.4 Calculations and Results

The evaluation of phase shifts and cross sections for the $^{12}C(p, p)^{12}C$ reaction by the IRM method requires a computer program which can accommodate a relatively complicated nuclear model and three or four open channels for each J^π over a wide energy range. For this purpose a computer code was developed on the basis of the experience gained in the solution of previous problems (*cf.* Chapters 4 and 5) together with the ideas involved in the related computer programs and numerical techniques[194,200-203]. The first phase of the program calculates the Racah and Clebsch-Gordan coefficients corresponding to a particular J^π and hence evaluates and stores the geometrical parts of the residual interaction mentioned in eqs. (6.3.18) and (6.3.19). This is followed by the calculation and storage of the form factors corresponding to the generalized Woods-Saxon potential [eq. (6.3.8)], the spin-orbit potential [eq. (6.3.1)] and the Coulomb interaction [eq. (6.3.12)] up to a radial distance much larger than the nuclear radius. The

TABLE (6.3.2): Geometrical parts of the matrix elements(*) of the residual interaction for $J^{\pi} = \frac{1}{2}^{+}$.

Configurations	$[0^{+} \otimes \frac{1}{2}]$	$[2^{+} \otimes \frac{3}{2}]$	$[2^{+} \otimes \frac{5}{2}]$
$[0^{+} \otimes \frac{1}{2}]$	0.00 (0.00)	0.00 (-0.28)	0.00 (0.35)
$[2^{+} \otimes \frac{3}{2}]$	0.00 (-0.28)	1.80 (0.20)	0.98 (-0.07)
$[2^{+} \otimes \frac{5}{2}]$	0.00 (0.35)	0.98 (-0.07)	-2.80 (0.23)

(*) In each block the upper number corresponds to the value of the quantities within the curly brackets in eq. (6.3.18), whereas that in parantheses corresponds to the same quantities in eq. (6.3.19).

TABLE (6.3.3): Same as table (6.3.2) but for $J^{\pi} = \frac{3}{2}^{+}$

Configurations	$[0^{+} \otimes \frac{3}{2}]$	$[2^{+} \otimes \frac{1}{2}]$	$[2^{+} \otimes \frac{3}{2}]$	$[2^{+} \otimes \frac{5}{2}]$
$[0^{+} \otimes \frac{3}{2}]$	0.00 (0.00)	0.00 (0.20)	0.00 (-0.20)	0.00 (-0.13)
$[2^{+} \otimes \frac{1}{2}]$	0.00 (0.20)	-3.00 (0.00)	0.00 (-0.20)	0.00 (-0.13)
$[2^{+} \otimes \frac{3}{2}]$	0.00 (-0.20)	0.00 (-0.20)	1.20 (0.00)	1.83 (-0.09)
$[2^{+} \otimes \frac{5}{2}]$	0.00 (-0.13)	0.00 (-0.13)	1.83 (-0.09)	-2.20 (0.08)

TABLE (6.3.4): Same as table (6.3.2) but for $J^{\pi} = \frac{5}{2}^{+}$

Configurations	$[0^{+} \otimes \frac{5}{2}]$	$[2^{+} \otimes \frac{1}{2}]$	$[2^{+} \otimes \frac{3}{2}]$	$[2^{+} \otimes \frac{5}{2}]$
$[0^{+} \otimes \frac{5}{2}]$	0.00 (0.00)	0.00 (0.20)	0.00 (0.11)	0.00 (-0.21)
$[2^{+} \otimes \frac{1}{2}]$	0.00 (0.20)	2.00 (0.00)	0.00 (0.11)	0.00 (-0.21)
$[2^{+} \otimes \frac{3}{2}]$	0.00 (0.11)	0.00 (0.11)	0.20 (-0.14)	2.40 (-0.04)
$[2^{+} \otimes \frac{5}{2}]$	0.00 (-0.21)	0.00 (-0.21)	2.40 (-0.04)	-1.20 (-0.14)

typical nature of the phenomenological form factor $f_2(r)$ [eq. (6.3.8)] was checked by comparing the results of the present calculations with those given by Mori and Terasawa[204].

The main part of the program is the computation of the basis set corresponding to the n.b.c. parameters in each channel. For closed channels these parameters are calculated at each energy by employing a subroutine for Whittaker functions and the definition (3.3.11) at the desired channel radius a_c. In order to ensure that this part of the program is correct, the results so obtained were compared with the tabulated values of Whittaker functions and their logarithmic derivatives at different ρ, η and l values[194]. These n.b.c. parameters for the closed channels together with arbitrary values for all except one, say k, of the open channels and an initial guess for the remaining open channel are used to solve the Schrödinger equation for the orthonormal basis states ϕ_j corresponding to the Hamiltonian H_0 of eq. (6.3.14) by using method VII of Fox and Goodwin[203]. These basis states are used to calculate the matrix elements of the residual interaction [i.e. eqs. (6.3.18) and (6.3.19)] and hence the elements of the R-matrix through the relation (3.4.9). Finally, the corresponding set of coupled-equations [Appendix (6.2A)] is solved to obtain the remaining phase shift and the relative amplitudes as discussed in the last section. This derived value of the phase shift is substituted into eq. (3.3.20) to determine a new value of the boundary condition parameter and the calculations are repeated with the corresponding basis states for the channel k. In this way an iteration procedure is formulated for each open channel. Generally one requires only two or three iterations per channel to ensure that the matrix elements $(T^{\pm})_{k'k}$ of eq. (6.2.14) correspond to the converged values of the n.b.c. parameters.

After performing various direct and indirect tests for checking the accuracy of different sections of the computer code, a relatively simplified form of the residual interaction (i.e. without including the spin-spin interaction, the energy-dependent term, the orbital angular momentum-dependent term and the quadrupole part of the Coulomb interaction) was used to calculate the phase shift $\delta^{+}_{\frac{1}{2}}$ and the inelasticity factor $\tau^{+}_{\frac{1}{2}}$ for the IRM method in the energy range below 8 MeV . The number of basis states was varied from two to four in each channel and several values of the channel radii were also tested. In each case the corresponding SRM calculations were significantly different from the IRM results.

At a later stage, the spin-spin interaction with the form factor $\tilde{f}_0(r)$ [eq. (6.3.16)] and the Coulomb potential with the form factor $f_{co(2)}(r)$ [eq. (6.3.12)] were introduced exactly. On the other hand, the effects of the energy-dependent term $\left(-a_E E_n\right)$ and the orbital angular momentum-dependent term $\left[(1.1)V_{ll}\right]$ could only be incorporated *approximately*(*) in the final calculations. This is apparently due to the inherent difference between the treatment of such state-dependent interactions in the coupled-

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(*) It may be worthwhile to elaborate the nature of these approximations at this stage. The interaction employed by Mikoshiba *et al.* appears to be slightly non-symmetric (and hence non-Hermitian) due to the presence of the state-dependent terms in the strength of the coupling potential. Whereas such potentials may be incorporated exactly in a straightforward coupled-channels calculation [e.g. numerically integrating the eq. (2.14) of ref.[70)]], none of the R-matrix type methods can accommodate them exactly due to the violation of the inherent requirements of symmetry in the overall formulation. This, in turn, implies that matrix elements of the residual interaction H_1 cannot be included exactly in the present IRM calculations. For example, it was not clear how to incorporate integrals like $\langle \phi_p | a_E (E_x - Q) | \phi_{p'} \rangle$ and $\langle \phi_p | (1.1) V_{ll} | \phi_{p'} \rangle$ exactly in the overall formulation. However, in order to keep the one-to-one correspondence between the present calculations and the coupled-channels results as close as possible, an approximate effect of the above mentioned quantities was taken into consideration. Since such approximations in the energy - and orbital angular momentum - dependent terms can give rise to a shift in the position of the resonances; one should expect some disagreement of the IRM method predictions with the coupled-channels results.

channels formulation[70] and the present approach. Moreover, instead of the power series expansion [eq. (6.3.4)] for the spin-orbit and Coulomb form factors[70], the expansion in spherical harmonics [eq. (6.3.7)] was used for these form factors in the overall formulation. *For these reasons, although the present calculations incorporate the model parameters of* Mikoshiba *et al.*[70] *the results are expected to differ slightly from the corresponding coupled-channels calculations.* With this prescription, the final calculations of the $\delta^{+}_{\frac{1}{2}}$ and $\tau^{+}_{\frac{1}{2}}$ by the IRM method incorporating the lowest four levels per channel were carried out for channel radii a_c = 6.0 fm(*). These results are shown in figure (6.4.1) where the corresponding SRM method results and the coupled-channels calculations[70] are also plotted. The agreement of the coupled-channels calculations with the experimental results is shown in figure (6.4.2) which is taken from the work of Mikoshiba *et al.*[70] It is apparent that the present IRM method calculations for $J^{\pi} = \frac{1}{2}^{+}$ reproduce almost exactly the corresponding coupled-channels calculations. The minor discrepencies may be due to the previously mentioned approximations in the nuclear model, differences in the fundamental constants and rounding off errors. The SRM calculations involving four levels per channel with $b_c = 0$ in all channels disagree significantly with these calculations. The results of some additional calculations have shown that whereas the IRM calculations have converged with four levels per channel, the SRM calculations with six levels per channel are still insufficient to reporduce the converged IRM results.

(*) It is not clear what values of the matching radii were used in the coupled-channels calculations of Mikoshiba *et al.*[70] In all the present calculations the value a_c = 6.0 fm was used although some test calculations have shown that the IRM results do not depend much on the choice of this parameter within the range $5.4 \leq a_c \leq 10.8$ fm .

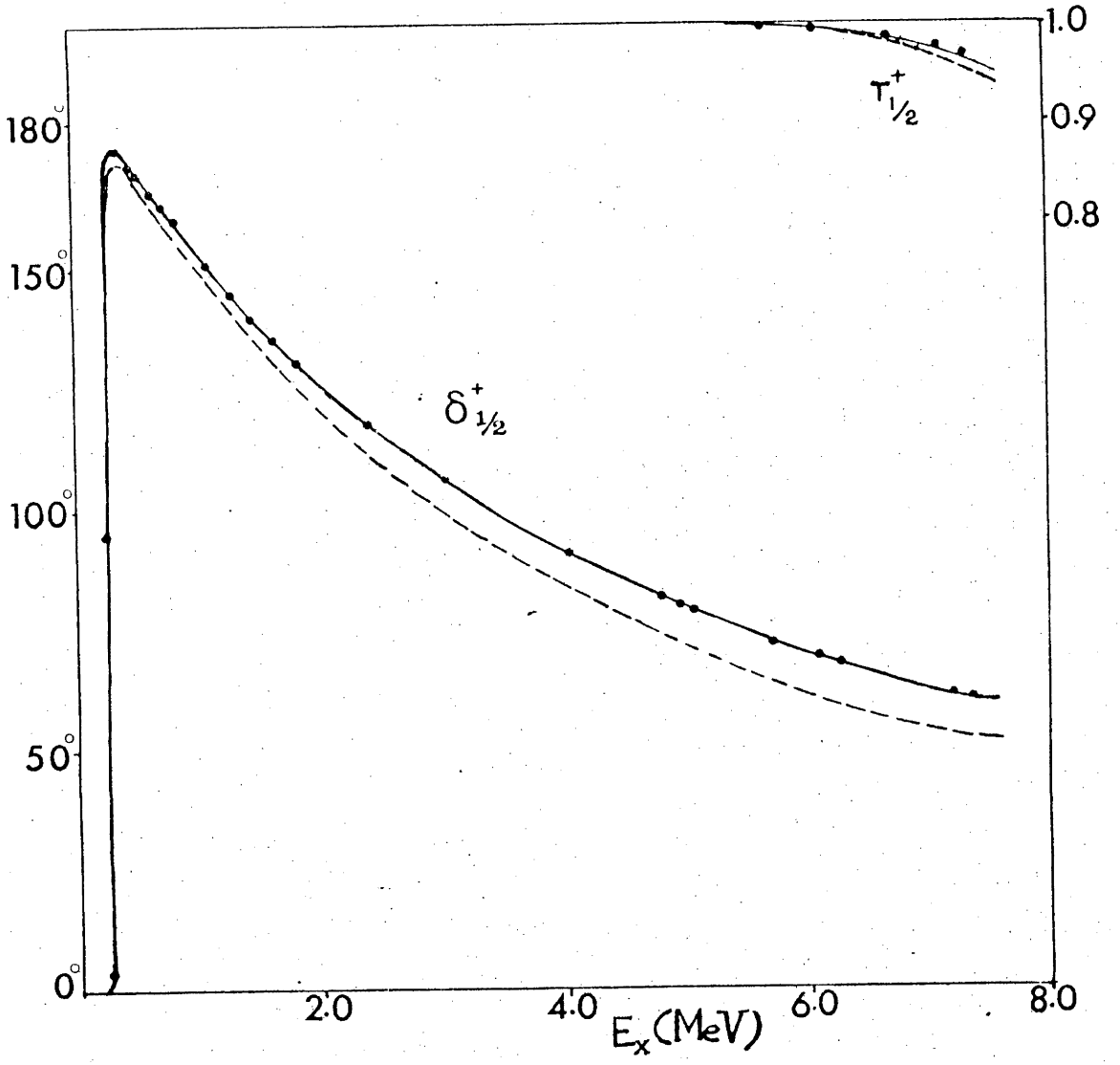

FIGURE (6.4.1): The $J^\pi = \frac{1}{2}^+$ phase shifts $\left(\delta^+_{\frac{1}{2}}\right)$ and inelasticity factors $\left(\tau^+_{\frac{1}{2}}\right)$ for the $^{12}C(p, p)^{12}C$ reaction using the IRM method (solid curve) with the lowest four levels per channel and the model parameters of table (6.3.1). The results are compared with the coupled-channels calculations (dots) of Mikoshiba *et al.*[70] and the corresponding SRM method calculations (dashed curve) with $b_c = 0$ in all channels.

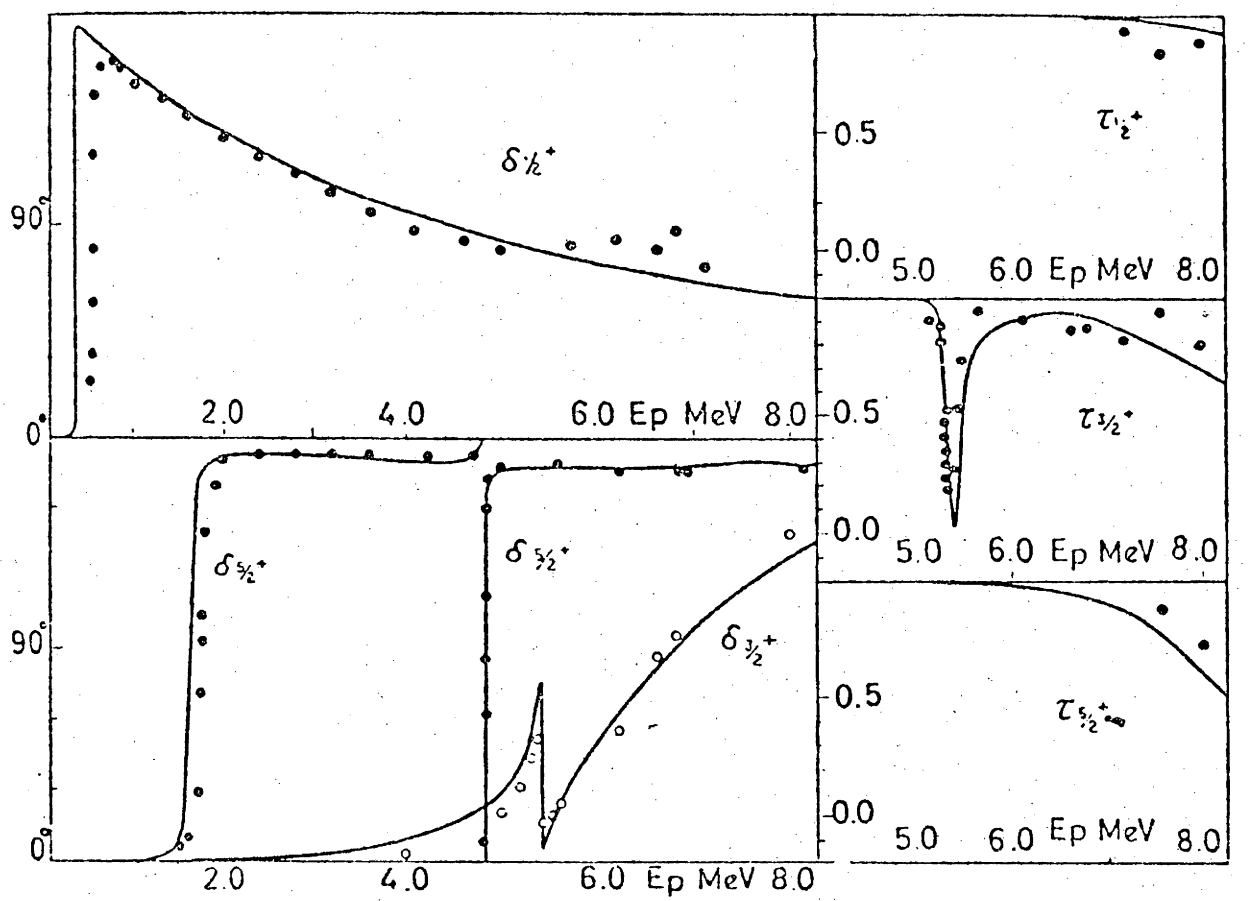

FIGURE (6.4.2): Comparison of the phase shifts (δ_{J^π}) and inelasticity factors (τ_{J^π}) corresponding to the J^π partial waves between the coupled-channels calculations of Mikoshiba *et al.*[70] (solid lines) and the phase shift analyses (dots and circles) of the data[62,205]. E_p represents the proton energy in the laboratory frame and further explanation of the symbols and notations is given in the text. The figure is reproduced from ref.[70].

The present results of the IRM and SRM calculations for $J^{\pi} = \frac{3}{2}^{+}$ and $\frac{5}{2}^{+}$ partial waves with the lowest four levels per channel are shown, respectively, in figures (6.4.3) and (6.4.4). Below the inelastic threshold, the IRM calculations for both $J^{\pi} = \frac{3}{2}^{+}$ and $\frac{5}{2}^{+}$ are generally in good agreement with the corresponding coupled-channels calculations. Apart from a 0.15 MeV shift in the position of the second $\frac{5}{2}^{+}$ resonance (dominant configuration $[2^{+} \otimes s_{\frac{1}{2}}]$), the phase shift corresponding to $J^{\pi} = \frac{5}{2}^{+}$ is quite well reproduced up to about $E_x = 7.2$ MeV . The corresponding inelasticity factor, $\tau^{+}_{\frac{5}{2}}$, disagrees considerably with the coupled-channels calculations and the possible reason for this discrepency will be discussed in the next section. The SRM calculations, with $b_c = 0$ in all channels, are not as satisfactory as the IRM calculations but tend to converge to the IRM results as the number of basis states in each channel is increased. This implies that in figure (6.4.4), the relatively improved position of the second $\frac{5}{2}^{+}$ resonance predicted by the SRM method with four levels per channel is not correct. Whereas the lowest four levels per channel in the IRM method are sufficient to reproduce satisfactorily the behaviour of $\delta^{+}_{\frac{3}{2}}$ phase shift up to about 5 MeV , the position of the broad $\frac{3}{2}^{+}$ resonance (mainly of configuration $[0^{+} \otimes d_{\frac{3}{2}}]$) is shifted by about 0.2 MeV . The possible reasons for this discrepency (and hence a corresponding difference in the phase shift within the energy region $E_x = 5.2 - 7.4$ MeV) will be discussed in the next section. It may be worth emphasizing here that this region is very sensitive to variations in the orbital angular momentum-dependent term of the residual interaction. Some test calculations have shown that a small change in the treatment of this term can give rise to significant changes in the overall results. However, the inelasticity factor $\tau^{+}_{\frac{3}{2}}$ is not influenced very much by such variations and the IRM calculations

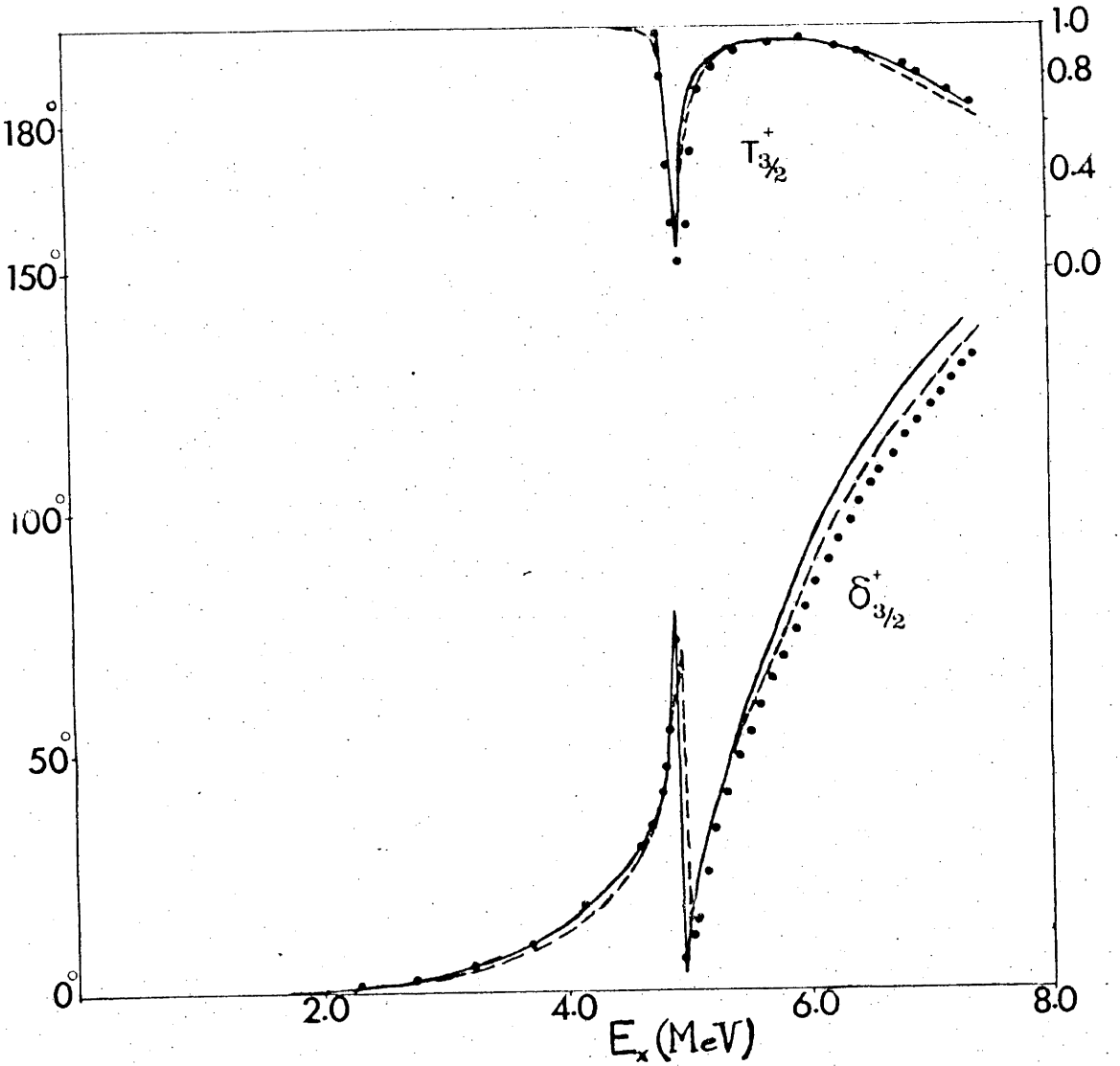

FIGURE (6.4.3): The $J^{\pi} = \frac{3}{2}^{+}$ phase shifts and inelasticity factors for the $^{12}C(p, p)^{12}C$ reaction. The SRM results converge to the IRM results by increasing the number of basis states in each channel. For further details see the caption of figure (6.4.1) and text.

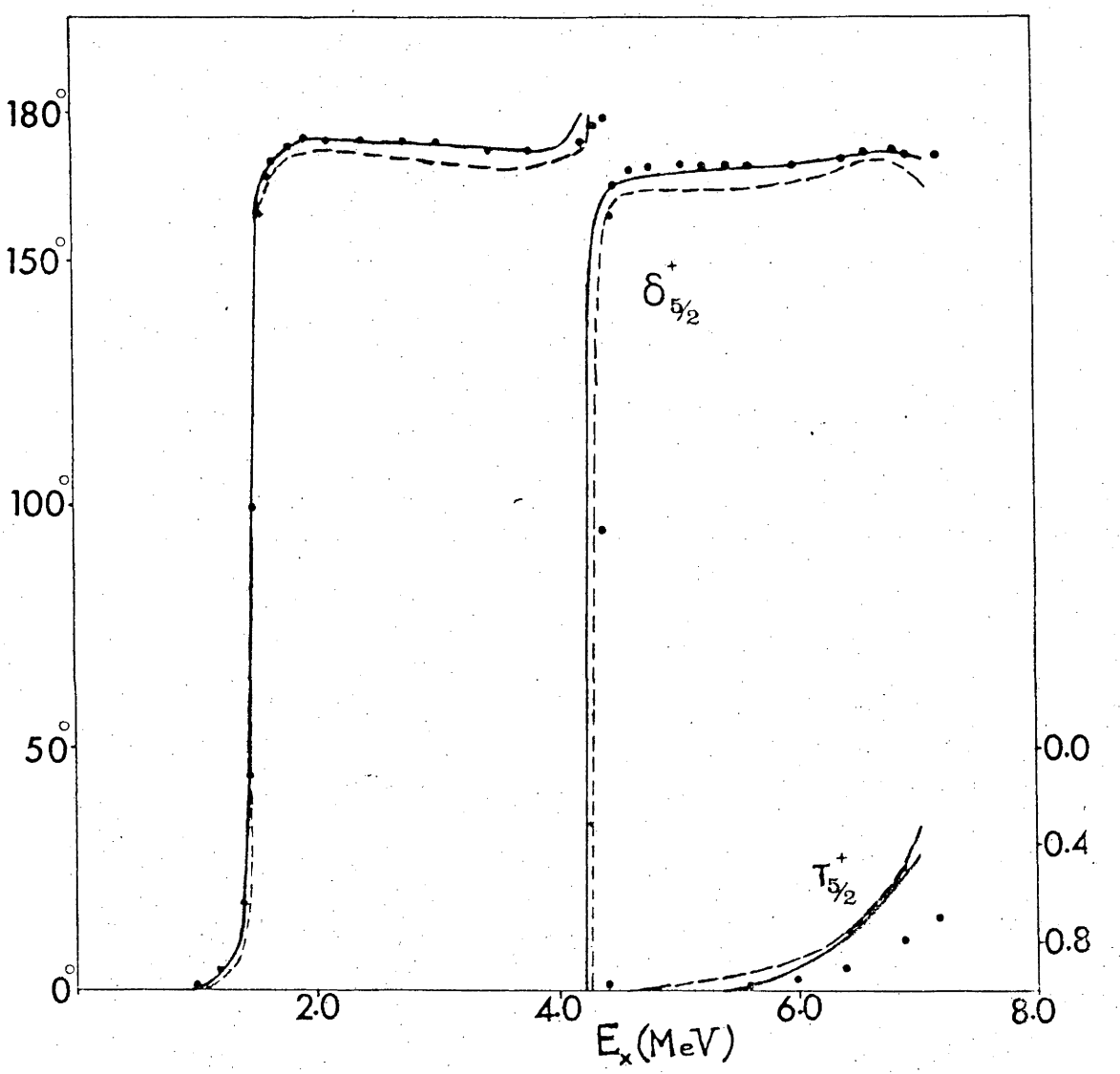

FIGURE (6.4.4): The $J^\pi = \frac{5}{2}^+$ phase shifts and inelasticity factors for the $^{12}C(p, p)^{12}C$ reaction. The SRM results converge to the IRM results by increasing the number of basis states in each channel. For further details see the caption of figure (6.4.1) and text.

reproduce this quantity very well over the entire energy region of interest. Again, the SRM calculations - involving the lowest four levels per channel and $b_c = 0$ in each channel - do not agree very well with the corresponding IRM calculations but do converge to the IRM results as the number of basis states is increased.

6.5 Discussion and Conclusion

The present work has shown that, given a realistic nuclear model, the IRM method can be successfully applied to calculate the cross sections and other observable quantities related to a nuclear reaction involving three and four open channels over a wide range of energy.

In order to study the $^{12}C(p, p)^{12}C$ reaction below 8 MeV, the present IRM calculations were carried out using a phenomenological nuclear model based upon the collective rotational model of Mikoshiba *et al.*[70] The main reason for this choice was that Mikoshiba *et al.* have employed their model in straightforward coupled-channels calculations for the $^{12}C(p, p)^{12}C$ reaction and - apart from a few minor discrepencies - their calculations reproduce exactly the corresponding experimental results. It was therefore considered that the employment of such a sophisticated nuclear model would be a real test of the reliability of the IRM method. Unfortunately, the inherent differences in the application of the two methods have inhibited the exact incorporation of the nuclear model in the present work. In fact, the computational form of the total Hamiltonian differs slightly from its original form. As discussed previously, these differences arise from the different treatments of the orbital angular momentum-dependent and the energy-dependent terms appearing in the strengths of the single particle and residual interactions.

The IRM calculations with four levels per channel have reproduced almost

exactly the coupled-channels calculations[70] for $\delta^{+}_{\frac{1}{2}}$ and $\tau^{+}_{\frac{1}{2}}$ over the whole energy region. The corresponding SRM calculations have been found to be unsatisfactory and may require eight or more levels per channel for convergence to the IRM results. For $J^{\pi} = \frac{1}{2}^{+}$ the coupled-channels calculations (and hence the IRM results) are in very good agreement with the phase shift analyses of the data [*cf.* figure (6.4.2)] except that the position of the $\frac{1}{2}^{+}$ resonance is about 0.2 MeV less than the observed value [*cf.* table (6.1.1)]. A similar disagreement is also found in the position of the first $\frac{5}{2}^{+}$ resonance predicted by the coupled-channels calculations[70]. In order to get these (potential) resonances at the right position, it was suggested[70] that an additional state-dependent potential should be added to the original potential. It has been speculated[206] that this requirement may be fulfilled by adding a term, say $+0.5\ \delta_{I_n,0}$ MeV (where I_n is the spin of ^{12}C state), to the strength $\tilde{V}_c$ [*cf.* eq. (6.3.17)] of the residual interaction. This term will shift the potential resonances $\frac{1}{2}^{+}$ and $\frac{5}{2}^{+}$ to higher energies by the desired amount and may also shift slightly the position of the second $\frac{3}{2}^{+}$ resonance(*) since such a potential will only influence the $[0^{+} \otimes j]$ configurations. It is intended to analyse the effects of including this term in additional IRM calculations to be carried out in the near future.

The IRM results for the $J^{\pi} = \frac{3}{2}^{+}$ phase shifts, with four levels per channel, are only marginally better than the corresponding SRM calculations(**) and both predictions are in very good agreement with the

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(*) The overall effect of this change in the position of $\frac{3}{2}^{+}$ resonance (dominant configuration $[0^{+} \otimes d_{\frac{3}{2}}]$) will not be so important because of the large width of the resonance.

(**) In this case the n.b.c. parameter for the open channel has a value close to that ($b_c = 0$) used in the SRM calculations.

coupled-channels results up to about 5 MeV . However, the position of the broad $\frac{3}{2}^+$ resonance is shifted by about 0.2 MeV and the phase shifts above 5 MeV are somewhat overestimated. The IRM predictions for the inelasticity factor $\tau_{\frac{3}{2}}^+$ agree very well with the coupled-channels calculations in the entire energy region of interest. Below 4.2 MeV , the IRM results with four levels per channel reproduce very well the $J^\pi = \frac{5}{2}^+$ phase shifts given by the coupled-channels method. Apart from a shift of about 0.15 MeV in the position of the second $\frac{5}{2}^+$ resonance, the behaviour of the IRM phase shifts is quite good in the remaining energy region. However, there is considerable disagreement between the prediction of the two methods for the inelasticity factors $\tau_{\frac{5}{2}}^+$ above 6 MeV . The SRM results with four levels per channel are quite unsatisfactory in the entire energy region but tend to converge to the IRM results as the number of basis states in each channel is increased. This establishes the reliability of the IRM method for a problem involving a sufficiently large number of open channels and a realistic nuclear model.

The possible reasons for the minor discrepencies between the IRM calculations and the corresponding coupled-channels results in certain energy regions will now be discussed. The main reason for these discrepencies seems to be due to the slightly different treatments of the energy-dependent and the orbital angular momentum-dependent terms in the nuclear Hamiltonian. Whereas the effect of the energy-dependent term is essentially to influence the position of the resonances relative to the ^{12}C states, the orbital angular momentum-dependent term adjusts the cross sections (and hence the phase shifts) in the inelastic region. Some test calculations have shown that the $J^\pi = \frac{3}{2}^+$ phase shifts are remarkably sensitive to minor variations in this term. Consequently, the coherent contributions arising from an improper employment of these terms in the nuclear potential - together with a possible difference in the fundamental constants - may give

a shift of ≈ 0.2 MeV in the positions of the $[\{0^+ \otimes d_{\frac{3}{2}}\}; \frac{3}{2}^+]$ and $[\{2^+ \otimes s_{\frac{1}{2}}\}; \frac{5}{2}^+]$ resonances and slightly overestimated values of $\delta^+_{\frac{3}{2}}$ and $\tau^+_{\frac{5}{2}}$ in the inelastic region. The reasons why $J^\pi = \frac{1}{2}^+$ phase shifts and inelasticity factors are not influenced by these differences are fairly obvious. First of all, there is no $\frac{1}{2}^+$ resonance in the corresponding inelastic region and hence the phase shifts and inelasticity factors are not as sensitive to the approximations in the coupling potential as in the $J^\pi = \frac{3}{2}^+$ and $\frac{5}{2}^+$ cases. Moreover, there are only three open channels corresponding to $J^\pi = \frac{1}{2}^+$ which are coupled by the nuclear potential and the orbital angular momentum-dependent term plays a less significant role. It is believed that the employment of a less sophisticated nuclear model (e.g. the rotational model used by Buttle[63] for the SRM and BCRM calculations) in the IRM method for the $^{12}C(p, p)^{12}C$ reaction will exactly reproduce the corresponding coupled-channels calculations.

It is intended to continue the present calculations in order to compare the predictions of the IRM method with the corresponding results of the BCRM method. Moreover, the IRM calculations for more sensitive observable quantities such as differential cross sections and polarizations at various energies of interest are already in progress. Finally, it is worth emphasizing that the coupled-channels calculations of Mikoshiba *et al.* do not take any account of the effect of antisymmetrization. Although it is not clear what would be the effect on their results of incorporating antisymmetrization; it is believed that in the NBC methods the use of antisymmetrized basis states may reduce the number of levels per channel required for an appropriate convergence. It may, therefore, be interesting to study this effect for the reaction under consideration.

CHAPTER 7

CONCLUSION

There have been several attempts during the last few decades to explain in a systematic way the occurrence of resonances in scattering and reaction cross sections. Although the *R*-matrix theory of nuclear reactions has been quite useful for parametrizing cross sections, most of the parameters involved do not have any particular physical significance. Hence an accurate *prediction* of the cross sections from an assumed underlying *physical model* is an important part of atomic, molecular and nuclear physics. In principle, the calculation can be carried out by the straightforward solution of the coupled integro-differential equations associated with the physical model, but this method is cumbersome when the model is sophisticated. For this reason, considerable attention has been given in recent years to alternative approaches to the problem. In view of its flexibility and the ease with which the basic ideas can be extended to the solution of similar problems in atomic and molecular physics(*), many of these approaches are connected in one way or another with the *R*-matrix theory of nuclear reactions.

In the standard *R*-matrix (SRM) method, the eigenstates of the total Hamiltonian are expanded in terms of a complete set of basis states. These states are taken to be the eigenstates of the *model* Hamiltonian in each channel within the internal region where all the channels are coupled through a *residual* interaction. For a truncated basis set, a diagonalization procedure enables one to determine the corresponding *R*-matrix and hence the cross sections. However, in some cases a satisfactory convergence requires

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(*) The *R*-matrix theory of atomic processes has been discussed thoroughly by Burke and Robb in a recent review article[207].

a large number of basis states. Two different approaches have been developed in order to overcome this problem. The first is the generalized *R*-matrix (GRM) method which essentially employs a more general form of basis states satisfying inhomogeneous boundary conditions at the surface of the internal region. The second approach is to try to include exactly the infinite basis set corresponding to the model Hamiltonian within the framework of the SRM method. The first successful step in this direction is the Buttle corrected *R*-matrix (BCRM) method which - in addition to the usual truncated basis set - analytically incorporates the effect of all the uncoupled levels in the corresponding infinite dimensional Hilbert space. However, the method is less effective when the coupling to and between the levels in the distant space becomes important. For such cases one may employ the variationally corrected *R*-matrix method which involves correcting a trial wave function (e.g. the BCRM method wave function) by accounting for the variations resulting from that part of the Hamiltonian which cannot be treated in the BCRM method. Although each of the *R*-matrix type methods is capable of reproducing the main features of the cross sections when a suitable model is available; none of the methods is free from problems especially when further details of the cross sections are to be predicted with a desirable accuracy.

The present thesis has dealt mainly with the development and application of two new methods for calculating reaction cross sections: the Barrett and Delsanto (BD) method and the iterative *R*-matrix (IRM) method. The development of these natural boundary condition (NBC) methods is based on the hypothesis that an optimum choice of boundary condition parameters and the employment of the most realistic physical model should minimize the number of basis states for achieving a desirable accuracy; especially in cases where the number of reaction channels is large. The first of the NBC methods to receive wide application for the calculation of reaction cross

sections was the eigenchannel method. Although this method is easily extendable to more complicated systems with sophisticated nuclear models, it is extremely wasteful numerically; involving many diagonalizations of large matrices. The BD method was developed in order to eliminate these numerical deficiencies and hence to drastically reduce the computing time involved. Starting from a division of configuration space into an external and an internal region in which all the polarizing interaction is assumed to occur, the BD method involves an iteration procedure in which the boundary conditions applied to the basis states are varied systematically until convergence to an optimum set of "natural boundary conditions" is obtained. While incorporating a matrix diagonalization technique similar to that used in the eigenchannel method, this method does not require the S-matrix to be obtained in a diagonal form and hence the overall calculation of the cross sections takes relatively less time for computation.

The IRM method may be regarded as a variant of the SRM method involving a matrix inversion technique but using an energy-dependent basis chosen by an iterative procedure. The R-matrix corresponding to the basis set satisfying the natural boundary conditions is used to calculate the S-matrix and associated cross sections in the standard way. This method resembles the BD method in the sense that both employ basis states which satisfy the natural boundary conditions. The main difference is in the numerical techniques: the BD method employs "matrix diagonalization" whereas the IRM method uses "matrix inversion" for determining the physical solutions of the nuclear Schrödinger equation. The results of the IRM method generally converge to the corresponding results of the BD method. Both the NBC methods do not lead automatically to an exactly symmetric and unitary S-matrix. This lack of symmetry is a distinct advantage since it gives an idea of the overall error in the calculation using a given truncated basis set. For practical purposes an exactly symmetric and unitary S-matrix can be obtained by a simple unitarization procedure.

It may be worth emphasizing that the two NBC methods only require a severely truncated set of basis states provided the strength of the coupling to and between different channels is not too strong. A large increase in the coupling strength gives rise to significant contributions from those levels belonging to that part of the function space outside the truncated basis. It has been found that a simple correction can be made to the energy eigenvalues and wave functions obtained from the BD method to allow approximately for the effect of these higher levels without increasing the dimensions of the matrices to be diagonalized. The effect of as many higher levels as necessary may be approximately included in the overall formulation, with a consequent improvement in the rate of convergence of the BD method. The possibility of a similar energy correction to the IRM method is under consideration.

In order to have an idea about the achievements and versatility of any new method, it is necessary to apply it to several realistic and model problems and compare the results with the equivalent existing methods.

In this spirit, the two NBC methods were first employed for the calculation of $^{12}C(n, n)^{12}C$ reaction cross section below the inelastic threshold of 4.43 MeV using the weak vibrational model of Reynolds *et al.*[66] and considering only the positive-parity states of the ^{13}C nucleus. Both methods have predicted two sharp resonances, a $\frac{5}{2}^+$ at 1.93 MeV and a $\frac{3}{2}^+$ at 2.77 MeV, superimposed upon a broad $\frac{3}{2}^+$ peak and a mainly s-wave background with two basis states per channel. The results are in good agreement with the observations and reproduce almost exactly the corresponding coupled-channels calculations of Reynolds *et al.* In calculating the $J^\pi = \frac{1}{2}^+$ and $\frac{3}{2}^+$ contribution to the total elastic cross section, the results of the NBC methods with only one basis state per channel agreed very well with the corresponding GRM results[75] with eight

harmonic oscillator basis states per channel. The NBC methods were also used for calculating the $J^{\pi} = \frac{3}{2}^{+}$ contribution to the total elastic cross section for a relatively stronger coupling potential. Comparison with the corresponding SRM calculations have shown that even four basis states per channel are insufficient to reproduce the NBC results with two levels per channel. The NBC methods were found to be independent of the channel radii within the range $6.0 \leq a_c \leq 12.0$ fm. The efficiency of each method depends very much on that part of the computer code which calculates the energy-dependent basis states. In all cases the two methods have given the same results, generally required few iterations to achieve a satisfactory result and converged very rapidly for an increase in the number of basis states.

After the successful application of the NBC methods to a realistic nuclear reaction problem essentially below the inelastic threshold, a further test of the reliability of these methods for the application to the important inelastic reactions with more than one open channel was also necessary. Furthermore, a systematic study of the effect of variations in the coupling strengths and channel radii for elastic as well as inelastic reactions can give further insight into the numerical accuracy of the methods together with the possibility of their successful application to atomic - and molecular - reaction problems. Since one of the best ways to compare the relative convergence of various methods in typical cases is to simulate a model problem for which the exact solution is known, the NBC methods were applied to an exactly soluble model comprising two square well potentials of strengths V_{11} and V_{22} coupled by a square well for various (i.e. weak, intermediate and strong) coupling strengths V_{12}. For the intermediate coupling case $\left(V_{12} = 1.072 \text{ MeV}, V_{11} = 32.161 \text{ MeV} \text{ and } V_{22} = 39.022 \text{ MeV}\right)$, the NBC methods with the lowest four levels per channel were compared with the exact and corresponding SRM and BCRM methods. It was

found that for values of the channel radii (7.5 fm) larger than the square well radii (6.0 fm), both the NBC and BCRM methods give a good description of the elastic and inelastic cross sections while the SRM calculations are quite poor. The results for the BD method including the energy correction with eight additional higher levels per channel were found to be indistinguishable from the exact calculations. When the coupling interaction was increased from 1.072 MeV to 20 MeV, the convergence of all methods was considerably worse. The NBC methods with the lowest six levels per channel give substantially better agreement with the exact results than either the SRM method or the BCRM method. Again the energy correction to the BD method, including the approximate effect of six higher levels per channel, gave results which were indistinguishable from the exact solution. Finally the NBC methods were tested for a typical weak coupling case[167] and the results compared with the corresponding one- and two-level approximations in the *R*-matrix theory[167] and the Kapur-Peierls dispersion theory[35,188]. These calculations show that the NBC methods with one level per channel lead to results at least as accurate as two-level *R*-matrix theory in a manner which can be applied to more realistic problems. Moreover, the calculation with essentially a two-level approximation in the Kapur-Peierls theory does not offer any significant advantage over the equivalent (one level per channel) NBC results and the theory suffers from the disadvantage of complex boundary condition parameters.

The above mentioned applications seem to lead the NBC methods to the stage where they can be tested further for more complicated but realistic cases incorporating, for example, many open channels, very sophisticated nuclear models, a Coulomb interaction and the effect of antisymmetrization. As a first step in this direction, one of the NBC methods (i.e. the IRM method) is applied to the $^{12}C(p, p)^{12}C$ reaction below 8 MeV by employing a nuclear model very similar to the macroscopic collective model of

Mikoshiba *et al.*[70] and without taking into consideration the negative parity states of the ^{13}N nucleus. The results of the phase shift analysis have shown that four basis states per channel in the IRM method are sufficient to reproduce almost exactly the phase shifts and the inelasticity factors for the $J^\pi = \frac{1}{2}^+$ partial wave obtained by the coupled-channels calculations of Mikoshiba *et al.* Whereas the shape and the positions of the resonances corresponding to $J^\pi = \frac{3}{2}^+$ and $\frac{5}{2}^+$ partial waves are also in satisfactory agreement, there is a slight quantitative disagreement of the resonance widths in the higher inelastic region which is not yet fully understood. This difference may be due to the approximations necessary for the incorporation of the nuclear model into the IRM formulation. The corresponding SRM results were often poor and in these cases convergence to the IRM results would probably require eight or more levels per channel. It is intended to continue the present calculations to test some possible improvements (e.g. employment of a prediagonalization procedure, an energy correction etc. etc.) to the IRM method. Moreover, some checks on the reliability of the method in connection with the evaluation of more sensitive observable quantities, such as angular distributions and polarizations for the $^{12}C(p, p)^{12}C$ reaction, are already in progress.

In conclusion, the two NBC methods discussed in the present work (in particular the energy corrected BD method) may be regarded as the most tractable approach for the practical calculation of reaction cross sections from a given physical model. This conclusion is emphasized in problems involving many channels and strong channel coupling. It is hoped that these methods will aid in the quest for a better understanding of the reaction processes in nuclear, atomic and molecular physics.

APPENDIX (2.2A1)

Since $GG^{-1} = G^{-1}G = 1$ by definition, one may write from eq. (2.2.6)

$$G^{-1} = \left(H+L(b)-E\right)$$

$$= H + \tilde{H} + L(\tilde{b}) - E$$

$$= H + \tilde{G}^{-1} \ , \qquad (2.2A.1)$$

where use has been made of the definitions (2.2.11) and (2.2.12). Writing

$$H = G^{-1} - \tilde{G}^{-1} \qquad (2.2A.2)$$

and considering the operator identity (assuming that each of the operators A and B has a definite inverse)

$$A^{-1} = B^{-1} + B^{-1}(B-A)A^{-1} = B^{-1} + A^{-1}(B-A)B^{-1} \ , \qquad (2.2A.3)$$

eq. (2.2A.2) may be written as

$$H = \tilde{G}^{-1}(\tilde{G}-G)G^{-1} \ ,$$

or

$$\tilde{G}H = (\tilde{G}-G)G^{-1} \ ,$$

or

$$\tilde{G}HG = \tilde{G} - G \ ,$$

i.e.

$$G = \tilde{G} - \tilde{G}HG \ , \qquad (2.2A.4)$$

as required by relation (2.2.13).

APPENDIX (2.2A2)

From eq. (2.2.19) one can write

$$\begin{aligned} \langle p|A|q\rangle &= \langle p|G^{-1}|q\rangle \\ &= \langle p|\left(H+L(b)-E\right)|q\rangle \\ &= \langle p|\left(H+\tilde{H}+L(\tilde{b})-E\right)|q\rangle \ , \end{aligned} \tag{2.2A.5}$$

where the last step is obtained by employing the relations (2.2.7), (2.2.8) and (2.2.12). Then

$$\begin{aligned} (A)_{pq} &= \langle p|H|q\rangle - E\delta_{pq} + \langle p|\tilde{H}+L(\tilde{b})|q\rangle \\ &= E_q\delta_{pq} - E\delta_{pq} + \langle p|H + L(\tilde{b})|q\rangle \\ &= \left(E_p-E\right)\delta_{pq} + \langle p|H|q\rangle \ , \end{aligned} \tag{2.2A.6}$$

since $L(\tilde{b})|q\rangle = 0$.

Finally, from the definitions (2.2.20), one gets the desired result

$$A = (B-E) \ . \tag{2.2A.7}$$

APPENDIX (2.2A3)

In order to prove that

$$S_{cc'} = i\hbar^{-1}\left[\langle O_{c'}|L(b^0)|I_c\rangle + \langle O_{c'}|L^*(b^0)-L(b^0)|\Psi\rangle\right] ,$$

one may proceed as follows.

Since the operator $L(b^0)$ annihilates the outgoing waves, i.e. $L(b^0)|O_c\rangle = 0$; the above equation can be written by employing the expansion (2.2.38) in the form

$$i\hbar S_{cc'} = \langle O_{c'}|L^*(b^0)|\Psi\rangle . \tag{2.2A.8}$$

Repeated use of the definitions and equations (2.2.4), (2.2.24), (2.2.38) and (2.2.39) enables one to evaluate the matrix element on the R.H.S. of eq. (2.2A.8); viz.

$$\text{R.H.S.} = \int_0^{a_{c''}} I_{c'} \sum_{c''} |\phi_{c''}) \frac{\hbar^2}{2\mu_{c''}a_{c''}} \left(\frac{d}{dr_{c''}} r_{c''} - b_{c''}^{0*}\right)(\phi_{c''}|\Psi\rangle\, \delta(r_{c''}-a_{c''}) r_{c''}^2 dr_{c''}$$

$$= \left[I_{c'} \sum_{c''} |\phi_{c''}) \frac{\hbar^2 a_{c''}}{2\mu_{c''}} \left\{\left(\frac{d}{dr} r - b_{c''}^{0*}\right)(\phi_{c''}|\Psi\rangle\right\}\right]_{r=a_{c''}} . \tag{2.2A.9}$$

The expression within the curly brackets may be evaluated as follows:

$$\{.\} = \left[\left(I'_{c'}\delta_{cc'}-S_{cc'}O'_{c'}\right)-\left(\frac{O'_{c''}}{O_{c''}}\right)^*\left(I_{c'}\delta_{cc'}-S_{cc'}O_{c'}\right)\right]V_{c'}^{-\frac{1}{2}}\delta_{c'c''}$$

$$= V_{c''}^{-\frac{1}{2}}I_{c''}^{-1}\left[I'_{c''}O_{c''}-I_{c''}O'_{c''}\right]_{r_{c''}=a_{c''}} S_{cc'}\delta_{c'c''}$$

$$= -2ik_{c''}V_{c''}^{-\frac{1}{2}}I_{c''}^{-1}S_{cc'}\delta_{c'c''} , \tag{2.2A.10}$$

where the prime denotes differentiation with respect to the radial coordinate and use has been made of the Wronskian relation at the surface,

$$W(I, O) = [IO'-OI'] \equiv 2ik . \tag{2.2A.11}$$

Substitution of eq. (2.2A.10) into eq. (2.2A.9) gives the result

$$\langle 0_{c'} | L^*(b^0) | \Psi \rangle = -i\hbar^2 k_{c''} S_{cc'} / \mu_{c''} V_{c''}$$

$$= -i\hbar S_{cc'} \,. \qquad (2.2A.12)$$

Q.E.D.

APPENDIX (2.5A)

In the zero coupling limit, i.e. $H_1 \equiv 0$ in eq. (2.3.17), the coupled R-matrix states $|\psi_\lambda\rangle$ - defined in eq. (2.3.8) - satisfy the relation

$$|\psi_\lambda^{(0)}\rangle = G^{(0)} L(b) |\psi_\lambda^{(0)}\rangle \tag{2.5A.1}$$

with

$$G^{(0)} = \left[H_0 + L(b) - E_\lambda^{(0)}\right]^{-1} \tag{2.5A.2}$$

in the usual notation. Using the analogue of expansion (2.3.16), e.g.

$$|\psi_\lambda^{(0)}\rangle = \sum_{p=1}^{\infty} C_{\lambda p}^{(0)} |p, c\rangle \ , \tag{2.5A.3}$$

it is straightforward to see that

$$C_{\lambda p}^{(0)} = \langle p, c | G^{(0)} L(b) | \psi_\lambda^{(0)}\rangle \ ; \tag{2.5A.4}$$

which in turn implies

$$\psi_{\lambda c}^{(0)}(r_c) = G(r_c, a_c)\left[a_c \frac{d\psi_{\lambda c}^{(0)}(r_c)}{dr_c} - b_c \psi_{\lambda c}^{(0)}(r_c)\right]_{r_c = a_c} \ , \tag{2.5A.5}$$

where, in the usual notation[18],

$$G(r_c, a_c) = \frac{\hbar^2}{2\mu_c a_c} \sum_{p=1}^{\infty} \frac{\omega_{pc}(r_c)\omega_{pc}(a_c)}{E_p^{(0)} - E_\lambda^{(0)}} \ , \tag{2.5A.6}$$

and use has been made of expansions similar to those in eqs. (2.2.41) and (2.2.42). Defining the channel R-function[18] as

$$R_{cc}^{(0)} = G(a_c, a_c) \ , \tag{2.5A.7}$$

and substituting into eq. (2.5A.5) gives the R-function in the form

$$R_{cc}^{(0)} = \left[\left\{r \frac{d}{dr}\left[\ln \psi_{\lambda c}^{(0)}(r)\right]\right\}_{r=a_c} - b_c\right]^{-1} \ , \tag{2.5A.8}$$

which can be calculated exactly, for a given b_c, by solving the

Schrödinger equation

$$\left(H_0 - E_\lambda^{(0)}\right) |\psi_\lambda^{(0)}\rangle = 0 \ . \qquad (2.5A.9)$$

Notice that the boundary condition parameter b_c in eq. (2.5A.8) is a fixed real number which may be obtained from[18]

$$b_c = \left[r \frac{d}{dr} \{ln\ \omega_{pc}(r)\} \right]_{r=a_c} ; \qquad (2.5A.10)$$

indicating that $L(b)|p, c\rangle = 0$. Moreover, the level-matrix character of $R_{cc}^{(0)}$, having a form similar to eq. (2.2.28), can be obtained by using the definition (2.5A.7).

APPENDIX (3.3A)

For N open channels, as discussed in Section 3.3, the nuclear Schrödinger eq. (3.3.2) assumes N degenerate solutions with an eigenvalue $E_i = E_x$ and one needs to determine N independent sets of phases δ_{kc}. For this purpose, one may assume some arbitrarily fixed boundary conditions for $c \neq k$ and vary δ_{kc} when $c = k$ for all k. For the sake of definiteness, consider the case $k = 1$ so that the phase δ_{11} may be searched in such a way that a solution of eq. (3.3.2) can be obtained for $E_i = E_x$.

Consider the set of equations (3.3.9) in the form

$$\sum_{j=1}^{\mu} \sum_{j=\mu+1}^{\nu} \left[(\varepsilon_j - E_i)\delta_{jk} + V_{kj}\right] a_{ij} = 0 \ , \qquad (3.3A.1)$$

where the first summation separates the μ equations corresponding to the boundary conditions specified by δ_{11} from the other $\nu-\mu$ equations that correspond to fixed boundary conditions. For further development it is convenient to rewrite the above set of equations by using the block matrices, viz.

$$\begin{pmatrix} P & V \\ V^{\dagger} & Q \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = E_x \begin{pmatrix} X \\ Y \end{pmatrix} \ ; \qquad (3.3A.2)$$

the quantities on the left hand side (L.H.S.) may be explained by writing

$$\text{L.H.S.} = \left[\begin{array}{cccc|cccc|c} \varepsilon_1+V_{11} & V_{12} & \cdots & V_{1\mu} & V_{1\eta} & V_{1\beta} & \cdots & V_{1\nu} & a_{11} \\ V_{21} & \varepsilon_2+V_{22} & \cdots & V_{2\mu} & V_{2\eta} & V_{2\beta} & \cdots & V_{2\nu} & a_{12} \\ \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots & \vdots \\ V_{\mu 1} & V_{\mu 2} & \cdots & \varepsilon_\mu+V_{\mu\mu} & V_{\mu\eta} & V_{\mu\beta} & \cdots & V_{\mu\nu} & a_{1\mu} \\ \hline & & & & \varepsilon_\eta+V_{\eta\eta} & V_{\eta\beta} & \cdots & V_{\eta\nu} & a_{1\eta} \\ & & & & V_{\beta\eta} & \varepsilon_\beta+V_{\beta\beta} & \cdots & V_{\beta\nu} & a_{1\beta} \\ & & V^\dagger & & \vdots & \vdots & & \vdots & \vdots \\ & & & & V_{\nu\eta} & V_{\nu\beta} & \cdots & \varepsilon_\nu+V_{\nu\nu} & a_{1\nu} \end{array}\right] \qquad (3.3A.3)$$

where $\dagger$ represents the adjoint of corresponding matrix and $\eta \equiv \mu+1$ and $\beta \equiv \mu+2$.

The basic idea is to *prediagonalize* the block matrix Q . Starting from the transformation

$$Y = CZ \ , \qquad (3.3A.4)$$

where C is a unitary matrix, one can write

$$C^\dagger QC = \Lambda \ , \qquad (3.3A.5)$$

where the elements of the diagonalized matrix Λ are such that

$$\Lambda_{ij} = \lambda_i \delta_{ij} \ . \qquad (3.3A.6)$$

With some straightforward matrix algebra, it is easy to show that the original set of equations in (3.3A.2) can be written as

$$PX + WZ = E_x X \ , \qquad (3.3A.7')$$

$$W^\dagger X + \Lambda Z = E_x Z \ , \qquad (3.3A.7'')$$

where

$$W = VC \ . \qquad (3.3A.8)$$

The equation (3.3A.7") leads to the transformed eigenvectors Z , i.e.

$$fZ = UW^\dagger X \qquad (3.3A.9)$$

where the matrix U is such that

$$U_{ij} = \frac{f\delta_{ij}}{E_x - \lambda_i} = \prod_{k\neq i} (E_x - \lambda_k)\delta_{ij} \ , \qquad (3.3A.10)$$

and the factor

$$f = \prod_k (E_x - \lambda_k) \qquad (3.3A.11)$$

is introduced in order to take care of the possibility that one of the λ_k coincides with E_x .

With this prescription, one can write eq. (3.3A.7') in the form

$$\left[f(P - IE_x) + WUW^{\dagger}\right] X = 0 \ , \qquad (3.3A.12)$$

where I is the identity matrix and the matrix within the square brackets is a $\mu \times \mu$ matrix. The above system of equation admits non-zero solutions only if

$$\det\left[f(P - IE_x) + WUW^{\dagger}\right] = 0 \ . \qquad (3.3A.13)$$

Notice that the last equation is equivalent to eq. (3.3.10) but it involves only the calculation of a very small determinant of dimension μ . Thus for each desired solution of eq. (3.3.2) the diagonalization of a large matrix meeds to be performed only once [i.e. eq. (3.3A.5)] and need not be repeated each time for different excitation energies E_x .

The search procedure is carried out by varying the phase δ_{11} and calculating the determinants in eq. (3.3A.13) of only that part of the matrix directly related with this phase. Finally, when eq. (3.3A.13) is satisfied, the eigenvectors [and hence the expansion coefficients of eq. (3.3.6)] are determined through eqs. (3.3A.4) and (3.3A.9), viz.

$$Y = \frac{1}{f} CU(VC)^{\dagger} X \ . \qquad (3.3A.14)$$

APPENDIX (3.4A)(*)

Given a matrix S , which is approximately symmetric and unitary, then the associated matrix

$$U = (I-S)(I+S)^{-1} , \tag{3.4A.1}$$

where I is the corresponding unit matrix, is approximately symmetric and anti-Hermitian, i.e.

$$U^{\dagger} \simeq -U . \tag{3.4A.2}$$

A matrix $\overline{U}$, which is *exactly* symmetric, anti-Hermitian and approximately equal to U , is given by

$$\overline{U} = \tfrac{1}{4}\left[U+U^{T}-U^{*}-U^{\dagger}\right] , \tag{3.4A.3}$$

where U^{T}, U^{*}, $U^{\dagger}$ are the transpose, complex conjugate and Hermitian conjugate (adjoint) of U , respectively. Then the associated matrix

$$\overline{S} = (I-\overline{U})(I+\overline{U})^{-1} \tag{3.4A.4}$$

is *exactly* symmetric, unitary and approximately equal to the original matrix S .

(*) The author is grateful to Dr R.J. Baxter for suggesting this unitarization procedure.

APPENDIX (4.2A)

From definitions (4.2.1) and (4.2.9), one can write

$$\langle (l'j'I')JM_J|H_1|(ljI)JM_J\rangle$$

$$= (\mathrm{GP})i^{l-l'}R_0V\int_0^\infty \omega_{p'c'}(r)\left[\frac{dg(r)}{dr}\right]\omega_{pc}(r)dr \ , \quad (4.2A.1)$$

where

$$(\mathrm{GP}) = -\langle l'j'I'JM_J|\sum_{\lambda\mu}(-)^{\mu}\alpha_{\lambda-\mu}Y_{\lambda\mu}(\hat{r})|ljIJM_J\rangle$$

$$= (-)^{1+j'+I'-J+j+I-J}\sum_{\lambda}\langle I'l'j'JM_J|\alpha_\lambda.Y_\lambda|Iljm_J\rangle \ . \quad (4.2A.2)$$

The last step is necessary since α acts on the target states whereas Y is connected with the single particle states.

In view of the identity[44]

$$\langle \alpha_1 j_1\alpha_2 j_2 JM|\left(T_1^{(k)}.T_2^{(k)}\right)|\alpha_1'j_1'\alpha_2'j_2'J'M'\rangle = (-)^{j_2+J+j_1'}\begin{Bmatrix} j_1 & j_2 & J \\ j_2' & j_1' & k\end{Bmatrix}\langle \alpha_1 j_1\|T_1^{(k)}\|\alpha_1'j_1'\rangle$$

$$\langle \alpha_2 j_2\|T_2^{(k)}\|\alpha_2'j_2'\rangle\delta_{JJ'}\delta_{MM'} \ , \quad (4.2A.3)$$

the relation (4.2A.2) takes the form

$$(\mathrm{GP}) = (-)^{1+J+j+I'}\begin{Bmatrix} I' & j' & J \\ j & I & \lambda\end{Bmatrix}\langle I'\|\alpha_\lambda\|I\rangle\langle (l'\tfrac{1}{2})j'\|Y_\lambda\|(l\tfrac{1}{2})j\rangle \ . \quad (4.2A.4)$$

Defining the nuclear deformation parameter as

$$\beta_\lambda = \langle I'\|\alpha_\lambda\|I\rangle \ , \quad (4.2A.5)$$

and making use of the identity[44]

$$\langle \tfrac{1}{2}lj\|Y_k\|\tfrac{1}{2}l'j'\rangle = (-)^{j-\frac{1}{2}}\frac{\hat{j}\hat{j}'\hat{k}}{\sqrt{4\pi}}\begin{pmatrix} j & k & j' \\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}\tfrac{1}{2}\left[1+(-1)^{l+l'+k}\right] \ , \quad (4.2A.6)$$

it is straightforward to show that

$$(\mathrm{GP}) = \sum_\lambda (-)^{I'+J+\lambda-\frac{1}{2}}\frac{\hat{j}\hat{j}'\hat{\lambda}}{\sqrt{4\pi}}\begin{pmatrix} j' & \lambda & j \\ -\frac{1}{2} & 0 & \frac{1}{2}\end{pmatrix}\begin{Bmatrix} I' & j' & J \\ j & I & \lambda\end{Bmatrix}\theta\beta_\lambda$$

$$= \sum_\lambda (-)^{J+j}\frac{\hat{j}\hat{j}'\hat{\lambda}}{\sqrt{4\pi}}W(I'j'Ij|J\lambda)C(j'\lambda j|-\tfrac{1}{2}0-\tfrac{1}{2})\theta\beta_\lambda \quad (4.2A.7)$$

where $\theta = \frac{1}{2}\left[1+(-1)^{l+l'+\lambda}\right]$, and the $3j$ and $6j$ symbols have been transformed into the corresponding Clebsch-Gordan and Racah coefficients in the standard way[44].

Finally, the desired result [eq. (4.2.10)] can be obtained by substituting eq. (4.2A.7) into eq. (4.2A.1) and considering only the quadrupole deformations ($\lambda = 2$) with $\beta_2 \equiv \beta$.

APPENDIX (5.2A)

In this Appendix the exact solution of the coupled eqs. (5.2.4) will be discussed in detail. From the definition of the form factors [eq. (5.2.3)] and the symmetry of the coupling interaction, one can write for $r \leq R$,

$$u_1''(r) = -Au_1(r) + Bu_2(r) \ , \tag{5.2A.1a}$$

$$u_2''(r) = \bar{A}u_1(r) - \bar{B}u_2(r) \ , \tag{5.2A.1b}$$

where

$$\left.\begin{aligned} A &= \frac{2m}{\hbar^2}\left(E_x - V_{11}\right) \ , \quad \bar{A} = \frac{2m}{\hbar^2} V_{12} \\ B &= \frac{2m}{\hbar^2} V_{12} = \bar{A} \ , \quad \bar{B} = \frac{2m}{\hbar^2}\left(E_x - Q - V_{22}\right) \end{aligned}\right\} . \tag{5.2A.2}$$

Of course, for $r > R$, these equations reduce to the simple form

$$u_1''(r) + \frac{2m}{\hbar^2} E_x u_1(r) = 0 \ , \tag{5.2A.3a}$$

$$u_2''(r) + \frac{2m}{\hbar^2}\left(E_x - Q\right)u_2(r) = 0 \ . \tag{5.2A.3b}$$

In order to solve the coupled set of equations, multiply eq. (5.2A.1b) by an arbitrary constant μ and add to the other equation such that

$$\bar{u}''(r) = (-A + \mu\bar{A})\bar{u}(r) \ , \tag{5.2A.4}$$

where

$$\bar{u}(r) = u_1(r) + \mu u_2(r) \ , \tag{5.2A.5}$$

and the constant μ satisfies the equation

$$B\mu^2 + (\bar{B} - A)\mu - B = 0 \ . \tag{5.2A.6}$$

The immediate solution of eq. (5.2A.4) is simply

$$\bar{u}(r) = \bar{C}_1 e^{iKr} + \bar{C}_2 e^{-iKr} \ , \tag{5.2A.7}$$

with the arbitrary constants $\bar{C}_1$ and $\bar{C}_2$ and

$$K^2 = A - \mu\bar{A} \ . \qquad (5.2A.8)$$

The actual solutions can be determined by considering the solutions of eq. (5.2A.6); viz.

$$\mu_1 = \frac{-\bar{B}+A}{2B} + \left[\left(\frac{A-\bar{B}}{2B}\right)^2 + 1\right]^{\frac{1}{2}} , \qquad (5.2A.9a)$$

$$\mu_2 = \frac{-\bar{B}+A}{2B} - \left[\left(\frac{A-\bar{B}}{2B}\right)^2 + 1\right]^{\frac{1}{2}} , \qquad (5.2A.9b)$$

with

$$\mu_1\mu_2 = -1 \ . \qquad (5.2A.10)$$

Consider the following forms of the solution (5.2A.7),

$$\bar{U}_1(r) = C_1 e^{iK_1 r} + C_2 e^{-iK_1 r} , \qquad (5.2A.11a)$$

$$\bar{U}_2(r) = C_3 e^{iK_2 r} + C_4 e^{-iK_2 r} , \qquad (5.2A.11b)$$

with an obvious significance for the subscripts of K and C_1, C_2, C_3 and C_4 being the arbitrary constants.

A little algebra gives the solutions

$$U_1(r) = (\mu_2-\mu_1)^{-1}\left[C_1\mu_2 e^{iK_1 r} + C_2\mu_2 e^{-iK_1 r} - C_3\mu_1 e^{iK_2 r} - C_4\mu_1 e^{-iK_2 r}\right] , \qquad (5.2A.12a)$$

$$U_2(r) = (\mu_1-\mu_2)^{-1}\left[C_1 e^{iK_1 r} + C_2 e^{-iK_1 r} - C_3 e^{iK_2 r} - C_4 e^{-iK_2 r}\right] . \qquad (5.2A.12b)$$

Assuming $U_1(r)$ and $U_2(r)$ to be the standing wave solutions such that

$$U_1(0) = 0 \ , \quad U_2(0) = 0 \ , \qquad (5.2A.13)$$

the set of eqs. (5.2A.12) gives

$$\mu_2(C_1+C_2) - \mu_1(C_3+C_4) = 0 \ ,$$

and

$$C_1 + C_2 - C_3 - C_4 = 0 \ ,$$

which are satisfied if

$$C_1 = -C_2 \ , \tag{5.2A.14a}$$

$$C_3 = -C_4 \ , \tag{5.2A.14b}$$

so that

$$U_1(r) = \frac{2iC_1\mu_2}{\mu_2-\mu_1}\sin K_1 r - \frac{2iC_3\mu_1}{\mu_2-\mu_1}\sin K_2 r \ , \tag{5.2A.15a}$$

$$U_2(r) = \frac{2iC_1}{\mu_1-\mu_2}\sin K_1 r - \frac{2iC_3}{\mu_1-\mu_2}\sin K_2 r \ . \tag{5.2A.15b}$$

In order to determine the phase shifts and cross sections, these solutions and their derivatives are to be matched at the boundary $r = R$ with the corresponding quantities obtained from eqs. (5.2A.3). If $E_c = E_x - Q_c$ for channel c with $Q_1 = 0$ and $Q_2 = Q$; one can define the external solutions from eqs. (5.2A.3) so that

$$U_{qc}^{(ext)} = V_{qc}e^{-|k_c|r} \ , \text{ for } E_c < 0 \ , \tag{5.2A.16a}$$

$$= V_c^{-\frac{1}{2}}V_{qc}\sin(k_c r+\delta_{qc}) \ , \text{ for } E_c > 0 \ , \tag{5.2A.16b}$$

where δ_{qc} is the phase shift for channel c corresponding to a particular solution q , V_c is the velocity and $k_c^2 = 2mE_c/\hbar^2$. These solutions will be considered in detail now.

CASE I: $E_c > 0$

Starting from eqs. (5.2A.15), one has to consider two types of solutions corresponding to two different choices of the constants C_1 and C_3 .

(i) *For* $q = 1$, choose $C_3 = 0$, $C_1 = \frac{\mu_2-\mu_1}{2i}$; so that

$$U_{11}(r) = \mu_2 \sin K_1 r \ , \tag{5.2A.17a}$$

$$U_{12}(r) = -\sin K_1 r \ , \tag{5.2A.17b}$$

and from eq. (5.2A.16b);

$$u_{11}^{(ext)} = V_1^{-\frac{1}{2}} V_{11} \sin\left(k_1 R+\delta_{11}\right) , \tag{5.2A.18a}$$

$$u_{12}^{(ext)} = V_2^{-\frac{1}{2}} V_{12} \sin\left(k_2 r+\delta_{12}\right) . \tag{5.2A.18b}$$

Matching the *logarithmic derivatives* of the last two sets of equations at $r = R$, one gets,

$$\delta_{q\nu} = \tan^{-1}\left[\frac{k_\nu}{K_q} \tan\left(K_q R\right)\right] - k_\nu R . \tag{5.2A.19}$$

The matching of the *amplitudes* or wave functions gives

$$\left(\frac{V_2}{V_1}\right)^{\frac{1}{2}} \frac{V_{11}\sin\left(k_1 R+\delta_{11}\right)}{V_{12}\sin\left(k_2 R+\delta_{12}\right)} = -\mu_2 = \frac{V_{11}\sin\theta_{11}}{V_{12}\sin\theta_{12}} \left(\frac{V_2}{V_1}\right)^{\frac{1}{2}} , \tag{5.2A.20}$$

where

$$\theta_{q\nu} = \tan^{-1}\left[\frac{k_\nu}{K_q} \tan\left(K_q R\right)\right] . \tag{5.2A.21}$$

(ii) *For* $q = 2$, choose $C_1 = 0$, $C_3 = \frac{\mu_1-\mu_2}{2i}$; so that

$$u_{21}(r) = \mu_1 \sin\left(K_2 r\right) , \tag{5.2A.22a}$$

$$u_{22}(r) = -\sin\left(K_2 r\right) , \tag{5.2A.22b}$$

and correspondingly,

$$u_{21}^{(ext)}(r) = V_1^{-\frac{1}{2}} V_{21} \sin\left(k_1 r+\delta_{21}\right) , \tag{5.2A.23a}$$

$$u_{22}^{(ext)}(r) = V_2^{-\frac{1}{2}} V_{21} \sin\left(k_2 r+\delta_{22}\right) . \tag{5.2A.23b}$$

As in the previous case, the matching of logarithmic derivatives and wave functions at the boundary yields a relation analogous to eq. (5.2A.19) for the phases $\delta_{q\nu}$ and

$$\left(\frac{V_2}{V_1}\right)^{\frac{1}{2}} \frac{V_{21}\sin\theta_{21}}{V_{22}\sin\theta_{22}} = -\mu_1 , \tag{5.2A.24}$$

with

$$K_q \tan\theta_{q\nu} = k_\nu \tan\left(K_q R\right) . \tag{5.2A.25}$$

The above knowledge of the phases and amplitudes is sufficient to

determine the complete S-matrix, since from eqs. (3.3.19) and (3.4.16) one can write

$$S = (T^-)^{-1}(T^+) \ , \tag{5.2A.26}$$

where

$$T^{\pm}_{ij} = V_{ij}e^{\pm\delta_{ij}} \ . \tag{5.2A.27}$$

Finally

$$\begin{pmatrix} S_{11} & S_{12} \\ S_{21} & S_{22} \end{pmatrix} = \begin{pmatrix} T^-_{11} & T^-_{12} \\ T^-_{21} & T^-_{22} \end{pmatrix}^{-1} \begin{pmatrix} T^+_{11} & T^+_{12} \\ T^+_{21} & T^+_{22} \end{pmatrix}$$

$$= \Delta \begin{pmatrix} \left[V_{11}V_{22}e^{i(\delta_{11}-\delta_{22})} - V_{12}V_{21}e^{i(\delta_{21}-\delta_{22})}\right] & \left[2iV_{22}V_{12}\sin(\delta_{12}-\delta_{22})\right] \\ \left[2iV_{11}V_{21}\sin(\delta_{21}-\delta_{11})\right] & \left[V_{11}V_{22}e^{i(\delta_{22}-\delta_{11})} - V_{12}V_{22}e^{i(\delta_{12}-\delta_{21})}\right] \end{pmatrix} \tag{5.2A.28}$$

where

$$\Delta^{-1} = V_{11}V_{22}e^{-i(\delta_{11}+\delta_{22})} - V_{12}V_{21}e^{-i(\delta_{12}+\delta_{21})} \ . \tag{5.2A.29}$$

Hence the elastic and reaction cross sections may be determined by using eqs. (5.2.5) and (5.2.6).

CASE II: $E_c < 0$

Consider the following set of independent eigenfunctions:

$$u_{11}(r) = \mu_2 \sin(K_1 r) \ , \quad u_{12}(r) = -\sin(K_1 r) \ ,$$

$$u_{21}(r) = \mu_1 \sin(K_2 r) \ , \quad u_{22}(r) = -\sin(K_2 r) \ .$$

The asymptotic solutions to which these solutions should be matched have the following form

$$\psi_1 \sim V_1^{-\frac{1}{2}}V_{11} \sin(k_1 r+\delta_{11}) + A_1 e^{-k_2 r} + B_1 e^{k_2 r} \ , \tag{5.2A.30}$$

$$\psi_2 \sim V_2^{-\frac{1}{2}} V_{21} \sin(k_1 r + \delta_{21}) + A_2 e^{-k_2 r} + B_2 e^{k_2 r} , \qquad (5.2A.31)$$

where $k_2^2 = 2m(-E_2)/\hbar^2$.

Since B_1 and B_2 are non-zero, neither ψ_1 nor ψ_2 is a suitable solution for determining the elastic scattering phase. However, one can take a linear combination of ψ_1 and ψ_2 such that the coefficient of the $e^{k_2 r}$ term is zero. Thus, one such combination is

$$\psi_3 = B_2 \psi_1 - B_1 \psi_2 . \qquad (5.2A.32)$$

In order to determine the constants B_1 & B_2 , one may match $U_{12}(r)$ and its logarithmic derivative to the corresponding external solutions at $r = R$. Thus, matching the amplitudes

$$-\sin(K_1 R) = A_1 e^{-k_2 R} + B_1 e^{k_2 R} , \qquad (5.2A.33)$$

and matching the logarithmic derivatives

$$K_1 \cot(K_1 R) = k_2 \left(e^{k_2 R} - \frac{A_1}{B_1} e^{-k_2 R} \right) \Big/ \left(e^{k_2 R} + \frac{A_1}{B_1} e^{-k_2 R} \right) , \qquad (5.2A.34)$$

such that

$$\frac{A_1}{B_1} = e^{2k_2 R} [k_2 - K_1 \cot(K_1 R)] / [k_2 + K_1 \cot(K_1 R)] . \qquad (5.2A.35)$$

Substitution in eq. (5.2A.33) gives

$$B_1 = -\sin(K_1 R) [k_2 + K_1 \cot(K_1 R)] / 2k_2 e^{k_2 R} . \qquad (5.2A.36)$$

Now, B_2 can be determined in an exactly similar way by matching $U_{22}(r)$ and $U_{22}^{(\text{ext})}(r) = A_2 e^{-k_2 r} + B_2 e^{k_2 r}$; viz.

$$B_2 = -\sin(K_2 R) [k_2 + K_2 \cot(K_2 R)] / 2k_2 e^{k_2 R} . \qquad (5.2A.37)$$

The wave function $\psi_3 = B_2 \psi_1 - B_1 \psi_2$, where B_1 and B_2 are defined by

eqs. (5.2A.36) and (5.2A.37) - apart from a common factor $\left(-1/2k_2 e^{k_2 R}\right)$ - has the following component in the first channel:

$$U_1(r) = B_2 U_{11}(r) - B_1 U_{21}(r)$$

$$= B_2 \mu_2 \sin(K_1 r) - B_1 \mu_1 \sin(K_2 r) \ . \qquad (5.2A.38)$$

This should be matched with the $U_1^{(ext)}(r) = V_1^{-\frac{1}{2}} V_1 \sin(k_1 r + \delta)$. Thus the matching of logarithmic derivatives at $r = R$ gives

$$k_1 \cot(k_1 R + \delta) = \frac{K_1 B_2 \mu_2 \cos(K_1 R) - K_2 B_1 \mu_1 \cos(K_2 R)}{B_2 \mu_2 \sin(K_1 R) - B_1 \mu_1 \sin(K_2 R)}$$

$$= \Lambda \ , \qquad (5.2A.39)$$

and hence the elastic scattering phase shift is

$$\delta = -k_1 R + \tan^{-1}(k_1/\Lambda) \ . \qquad (5.2A.40)$$

The elastic scattering cross section is $\frac{4\pi}{k_1^2} \sin^2\delta$ and the reaction cross section is zero.

APPENDIX (5.3A)

The analytic calculation of the basis states for the BD and IRM methods will be discussed in this Appendix. For the system under consideration, the basis states are the solutions of the radial Schrödinger equation in each channel c ; viz.

$$\frac{d^2\phi_c}{dr^2} + \frac{2m}{\hbar^2}\left[E_c - V_c(r)\right]\phi_c = 0 \ , \tag{5.3A.1}$$

where

$$\left.\begin{aligned} V_c(r) &= -V \ , \quad r \le R \\ &= 0 \ , \quad r > R \end{aligned}\right\} \ , \tag{5.3A.2}$$

and E_c is the eigenenergy in each channel c . Two main cases (i.e. open and closed channels) will be dealt with explicitly.

CASE I: OPEN CHANNEL

The regular solution of eq. (5.3A.1) are

$$\phi_c(r) = A_c \sin\left(K_c r\right) \ ; \ r \le R \ , \tag{5.3A.3}$$

$$\phi_c(r) = B_c \sin\left(k_c r\right) \ ; \ r > R \ , \tag{5.3A.4}$$

where $K_c^2 = 2m\left[E_c - V_c(r)\right]\hbar^{-2}$ and $k_c^2 = 2mE_c/\hbar^2$. In order to determine the constants B_c and δ_c , the logarithmic derivatives and amplitudes should be matched at $r = R$; viz.

$$B_c = A_c \sin\left(K_c R\right)/\sin\left(k_c R + \delta_c\right) \ , \tag{5.3A.5}$$

and

$$\delta_c = \tan^{-1}\left[\frac{k_c}{K_c}\tan\left(K_c R\right)\right] - k_c R \ . \tag{5.3A.6}$$

The normalization constant is to be determined in the following way. Let a $(> R)$ be the matching radius then the normalization condition is

$$1 = \int_0^a \phi_c^2(r)dr$$

$$= A_c^2 \int_0^R \sin^2(K_c r)dr + \frac{A_c^2 \sin^2(K_c R)}{\sin^2[k_c R+\delta_c]} \int_R^a \sin^2(k_c r+\delta_c)dr$$

$$= A_c^2 \left[\frac{R}{2} - \frac{\sin(2K_c R)}{4K_c} + \frac{\sin^2(K_c R)}{\sin^2[k_c R+\delta_c]k_c} \int_{k_c R+\delta_c}^{k_c a+\delta_c} \sin^2 x dx\right] . \qquad (5.3A.7)$$

Some straightforward algebra gives

$$A_c^{-2} = \frac{R}{2} - \frac{\sin(2K_c R)}{4K_c} + \frac{\sin^2(K_c R)}{\sin^2[k_c R+\delta_c]}$$

$$\left\{\frac{a-R}{2} - \frac{1}{2k_c}\left[\sin(k_c a-k_c R)\cos(k_c a+k_c R+2\delta_c)\right]\right\} . \qquad (5.3A.8)$$

CASE II: CLOSED CHANNEL

Again, there are two solutions corresponding to internal and external regions, i.e.

$$\phi_c(r) = A \sin(K_c r) \; ; \quad r \le R , \qquad (5.3A.9)$$

$$\phi_c(r) = Ce^{-kr} + De^{kr} , \quad r > R , \qquad (5.3A.10)$$

with $k^2 = -2mE/\hbar^2$ and A, C, D being arbitrary constants. As before, the matching of the logarithmic derivatives and the amplitudes at the boundary $r = R$ gives the relations

$$\frac{C}{D} = \left[\frac{k-K_c \cot(K_c R)}{k+K_c \cot(K_c R)}\right] e^{2kR} , \qquad (5.3A.11)$$

$$D = A \sin(K_c R)\left[k+K_c \cot(K_c R)\right] e^{-kR}/2k , \qquad (5.3A.12)$$

$$C = A \sin(K_c R)\left[k-K_c \cot(K_c R)\right] e^{kR}/2k . \qquad (5.3A.13)$$

The constant A is to be determined by the normalization condition, i.e.

$$A^2 \int_0^R \sin^2(K_c r)dr + \int_R^a \left[Ce^{-kr}+De^{kr}\right]^2 dr = 1 . \qquad (5.3A.14)$$

Some straightforward but lengthy algebra finally gives the following result after making use of eqs. (5.3A.11)-(5.3A.13);

$$A^{-2} = \frac{R}{2} - \frac{\sin(2K_c R)}{4K_c} + \Big[\{1-e^{-2k(a-R)}\}\{k^2 \sin^2(K_c R) + K_c^2 \cos^2(K_c R) - 2kK_c \sin(K_c R)\cos(K_c R)\}$$
$$+ \{e^{2k(a-R)}-1\}\{k^2 \sin^2(K_c R) + K_c^2 \cos^2(K_c R) + 2kK_c \sin(K_c R)\cos(K_c R)\}\Big]/8k^3$$
$$+ (a-R)\{k^2 \sin^2(K_c R) - K_c^2 \cos^2(K_c R)\}/2k^2 \quad . \quad (5.3A.15)$$

APPENDIX (6.2A)

The purpose of this Appendix is to recapitulate the calculable forms of the sets of eqs. (3.4.17) for the $^{12}C+p$ system. Above the inelastic threshold (Case I), this system comprises at most four open channels within the framework of the formulation developed in Section 6.2. Below the inelastic threshold (Case II), there is only one open channel and at most three closed channels. These cases are discussed below.

CASE I. In order to make the presentation as compact as possible, the following notations and symbols will be adopted:

$$\tilde{V}_{k'c'} = V_{k'c'}/V_{k'k'} \sin \tilde{\delta}_{k'k'} ,$$

$$V_{k'c'} = (V_{k'}/V_{c'})^{\frac{1}{2}} ,$$

$$\tilde{\delta}_{c'c'} = \delta_{k'c'} - \omega_{c'} ,$$

$$X_{c'k'c'} = V_{k'c'}[F'_{c'} \cos \tilde{\delta}_{k'c'} + G'_{c'} \sin \tilde{\delta}_{k'c'}] ,$$

$$X'_{c'k'c'} = V_{k'c'}[F'_{c'} \cos \tilde{\delta}_{k'c'} + G'_{c'} \sin \tilde{\delta}_{k'c'}] ,$$

where the amplitudes $V_{k'c'}$ and the phases $\delta_{k'c'}$ are defined in eq. (6.2.13) and the rest of the symbols have obvious significance with reference to the context of Sections 3.4 and 6.2. The resulting set of equations for each solution $\chi_{k'}$ $(k' = 1, \ldots, 4)$ are summarized in relations (6.2A.1)-(6.2A.4).

CASE II. All symbols have their usual significance in this case except that the Whittaker function is replaced by the quantity $iH^-_{c'}$. The only set of equations corresponding to χ_1 is given through the relation (6.2A.5).

$$\begin{bmatrix} R_{11}F'_1 - a_1^{-1}F_1 & R_{12}X'_{212} & R_{13}X'_{313} & R_{14}X'_{414} \\ R_{21}F'_1 & R_{22}X'_{212} - a_2^{-1}X_{212} & R_{23}X'_{313} & R_{24}X'_{414} \\ R_{31}F'_1 & R_{32}X'_{212} & R_{33}X'_{313} - a_3^{-1}X_{313} & R_{34}X'_{414} \\ R_{41}F'_1 & R_{42}X'_{212} & R_{43}X'_{313} & R_{44}X'_{414} - a_4^{-1}X_{414} \end{bmatrix} \begin{bmatrix} \cot\tilde{\delta}_{11} \\ I\!V_{12} \\ I\!V_{13} \\ I\!V_{14} \end{bmatrix} = \begin{bmatrix} -R_{11}G'_1 + a_1^{-1}G_1 \\ -R_{21}G'_1 \\ -R_{31}G'_1 \\ -R_{41}G'_1 \end{bmatrix} \tag{6.2A.1}$$

$$\begin{bmatrix} R_{11}X'_{121} - a_1^{-1}X_{121} & R_{12}F'_2 & R_{13}X'_{323} & R_{14}X'_{424} \\ R_{21}X'_{121} & R_{22}F'_2 - a_2^{-1}F_2 & R_{23}X'_{323} & R_{24}X'_{424} \\ R_{31}X'_{121} & R_{32}F'_2 & R_{33}X'_{323} - a_3^{-1}X_{323} & R_{34}X'_{424} \\ R_{41}X'_{121} & R_{42}F'_2 & R_{43}X'_{323} & R_{44}X'_{424} - a_4^{-1}X_{424} \end{bmatrix} \begin{bmatrix} I\!V_{21} \\ \cot\tilde{\delta}_{22} \\ I\!V_{23} \\ I\!V_{24} \end{bmatrix} = \begin{bmatrix} -R_{21}G'_2 \\ -R_{22}G'_2 + a_2^{-1}G_2 \\ -R_{32}G'_2 \\ -R_{42}G'_2 \end{bmatrix} \tag{6.2A.2}$$

$$\begin{bmatrix} R_{11}X'_{131} - a_1^{-1}X_{131} & R_{12}X'_{232} & R_{13}F'_3 & R_{14}X'_{434} \\ R_{21}X'_{131} & R_{22}X'_{232} - a_2^{-1}X_{232} & R_{23}F'_3 & R_{24}X'_{434} \\ R_{31}X'_{131} & R_{32}X'_{232} & R_{33}F'_3 - a_3^{-1}F_3 & R_{34}X'_{434} \\ R_{41}X'_{131} & R_{42}X'_{232} & R_{43}F'_3 & R_{44}X'_{434} - a_4^{-1}X_{434} \end{bmatrix} \begin{bmatrix} I\!V_{31} \\ I\!V_{32} \\ \cot\tilde{\delta}_{33} \\ I\!V_{34} \end{bmatrix} = \begin{bmatrix} -R_{13}G'_3 \\ -R_{23}G'_3 \\ -R_{33}G'_3 + a_3^{-1}G_3 \\ -R_{43}G'_3 \end{bmatrix} \tag{6.2A.3}$$

$$\begin{bmatrix} R_{11}X'_{141} - a_1^{-1}X_{141} & R_{12}X'_{242} & R_{13}X'_{343} & R_{14}F'_4 \\ R_{21}X'_{141} & R_{22}X'_{242} - a_2^{-1}X_{242} & R_{23}X'_{343} & R_{24}F'_4 \\ R_{31}X'_{141} & R_{32}X'_{242} & R_{33}X'_{343} - a_3^{-1}X_{343} & R_{34}F'_4 \\ R_{41}X'_{141} & R_{42}X'_{242} & R_{43}X'_{343} & R_{44}F'_4 - a_4^{-1}F_4 \end{bmatrix} \begin{bmatrix} \overline{V}_{41} \\ \overline{V}_{42} \\ \overline{V}_{43} \\ \cot\tilde{\delta}_{44} \end{bmatrix} = \begin{bmatrix} -R_{14}G'_4 \\ -R_{24}G'_4 \\ -R_{34}G'_4 \\ -R_{44}G'_4 + a_4^{-1}G_4 \end{bmatrix} \tag{6.2A.4}$$

$$\begin{bmatrix} V_1^{-\frac{1}{2}}\left(R_{11}F'_1 - a_1^{-1}F_1\right) & R_{12}H'_2 & R_{13}H'_3 & R_{14}H'_4 \\ V_1^{-\frac{1}{2}}R_{21}F'_1 & R_{22}H'_2 - a_2^{-1}H_2 & R_{23}H'_3 & R_{24}H'_4 \\ V_1^{-\frac{1}{2}}R_{31}F'_1 & R_{32}H'_2 & R_{33}H'_3 - a_3^{-1}H_3 & R_{34}H'_4 \\ V_1^{-\frac{1}{2}}R_{41}F'_1 & R_{42}H'_2 & R_{43}H'_3 & R_{44}H'_4 - a_4^{-1}H_4 \end{bmatrix} \begin{bmatrix} \cot\tilde{\delta}_{11} \\ \overline{V}_{12} \\ \overline{V}_{13} \\ \overline{V}_{14} \end{bmatrix} = \begin{bmatrix} \left(-R_{11}G'_1 + a_1^{-1}G_1\right)V_1^{-\frac{1}{2}} \\ -R_{21}G'_1V_1^{-\frac{1}{2}} \\ -R_{31}G'_1V_1^{-\frac{1}{2}} \\ -R_{41}G'_1V_1^{-\frac{1}{2}} \end{bmatrix}$$

(6.2A.5)

APPENDIX (6.3A1)

From eq. (6.3.15) and the definition of basis states ϕ_j, one can write

$$\langle \phi_p, |\overline{H}_1| \phi_p \rangle = \langle (l'j'I')J'M_J, |V_{\sigma I}(\sigma.\mathrm{I})\tilde{f}_0(r)|(ljI)JM_J\rangle$$

$$= (\mathrm{M.E.})i^{l-l'}V_{\sigma I}\int_0^\infty \omega_{p'c'}(r)\tilde{f}_0(r)\omega_{pc}(r)dr \ , \qquad (6.3A.1)$$

with

$$(\mathrm{M.E.}) = \langle \alpha' j' m_j, I'M_I, J'M_J, |(\sigma.\mathrm{I})|\alpha j m_j IM_I JM_J\rangle$$

$$= (-1)^{I'+J'+j}\begin{Bmatrix} j' & I' & J' \\ I & j & 1 \end{Bmatrix}\langle \alpha' j' \|\sigma\|\alpha j\rangle\langle I'\|\mathrm{I}\|I\rangle\delta_{JJ'}\delta_{M_J M_{J'}}, \qquad (6.3A.2)$$

where use has been made of the identity in eq. (4.2A.3). Moreover, one can write

$$\langle \alpha' j' \|\sigma|\alpha j\rangle = \langle l'\tfrac{1}{2}j'\|\sigma\|l\tfrac{1}{2}j\rangle$$

$$= (-1)^{l'+\frac{1}{2}+j'+1}\hat{j}'\hat{j}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ j & j' & l' \end{Bmatrix}\langle \tfrac{1}{2}\|\sigma\|\tfrac{1}{2}\rangle\delta_{ll'} \ . \qquad (6.3A.3)$$

The last relation is a consequence of the identity[44],

$$\langle j_1 j_2 J\|T^{(k)}(2)\|j_1' j_2' J'\rangle = (-1)^{j_1+j_2'+J+k}\hat{j}\hat{j}'\begin{Bmatrix} j_2 & j_2' & k \\ J' & J & j_1 \end{Bmatrix}$$

$$\langle j_2\|T^{(k)}(2)\|j_2'\rangle\delta_{j_1 j_1'} \ . \qquad (6.3A.4)$$

Since

$$\langle \tfrac{1}{2}\|\sigma\|\tfrac{1}{2}\rangle = \sqrt{\sigma(\sigma+1)}\hat{\sigma} = \sqrt{6} \ , \qquad (6.3A.5)$$

and

$$\langle I'\|\mathrm{I}\|I\rangle = \sqrt{I(I+1)}\hat{I}\delta_{II'} \ ; \qquad (6.3A.6)$$

the substitution of above relations in eq. (6.3A.2) gives

$$(\text{M.E.}) = (-1)^{\frac{3}{2}+l'+j+j'+I'+J'}\sqrt{6I(I+1)}\hat{j}\hat{j}'\hat{I}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & 1 \\ j & j' & l' \end{Bmatrix}$$

$$\begin{Bmatrix} j' & I' & J' \\ I & j & 1 \end{Bmatrix}\delta_{ll'}\delta_{II'}\delta_{M_JM_{J'}}\delta_{JJ'} \ . \qquad (6.3A.7)$$

Finally, the desired result [eq. (6.3.18)] can be obtained by transforming the $6j$-symbols in the above equation into Racah coefficients and substituting the results in eq. (6.3A.1).

APPENDIX (6.3A2)

Starting from eq. (6.3.15), one can write

$$\langle \phi_{p'} | \tilde{H}_1 | \phi_p \rangle = \sum_{\lambda \neq 0} (\text{M.E.}) i^{l-l'} (4\pi)^{\frac{1}{2}} / \hat{\lambda}$$

$$\int_0^\infty \omega_{p'c'}(r) \left[\tilde{V}_c f_\lambda(r) + \sqrt{4\pi} \xi f_{co(\lambda)} \right] \omega_{pc}(r) dr \ , \qquad (6.3A.8)$$

with

$$(\text{M.E.}) = \langle (l'j'I')J'M_{J'} | \Omega | (ljI)JM_J \rangle \ , \qquad (6.3A.9)$$

such that

$$\Omega = \frac{\hat{\lambda}}{(4\pi)^{\frac{1}{2}}} \sum_\mu D^\lambda_{\mu 0}(\alpha\beta\gamma) Y_{\lambda\mu}(\theta, \phi)$$

$$= \sum_\mu Y^*_{\lambda\mu}(\beta\alpha) Y_{\lambda\mu}(\theta, \phi)$$

$$= \sum_\mu (-)^\mu Y_{\lambda\mu}(\theta, \phi) Y_{\lambda, -\mu}(\beta\alpha) \ , \qquad (6.3A.10)$$

where use has been made of several transformation properties of the spherical harmonics and the rotation matrices[195] with Euler angles α, β, γ . In view of the definition of the contraction of two irreducible tensors having equal rank L ; viz.[195]

$$T^L(1).T^L(2) = \sum_M (-)^M T_{LM}(1) T_{L,-M}(2) \ , \qquad (6.3A.11)$$

eq. (6.3A.9) takes the form

$$(\text{M.E.}) = \langle l'\tfrac{1}{2}j'; I', JM_J | Y^\lambda(\theta, \phi).Y^\lambda(\beta\alpha) | l\tfrac{1}{2}j; I, JM_J \rangle$$

$$= (-1)^{I'+J+j} \begin{Bmatrix} j' & I' & J \\ I & j & \lambda \end{Bmatrix} \langle l'\tfrac{1}{2}j' \| Y^\lambda \| l\tfrac{1}{2}j \rangle \langle I' \| Y^\lambda \| I \rangle \ , \qquad (6.3A.12)$$

where the last relation is obtained by using the identity (4.2A.3). The reduced matrix elements in the above equation can be evaluated by using the relation (6.2A.6) and similar formulae[44]; viz.

$$\langle l'\tfrac{1}{2}j'\|Y^{\lambda}\|l\tfrac{1}{2}j\rangle = (-1)^{l'+l-j+\frac{1}{2}}\tfrac{1}{2}\left[1+(-1)^{l'+l+\lambda}\right]\frac{\hat{j}\hat{\lambda}\hat{j}'}{(4\pi)^{\frac{1}{2}}}\begin{pmatrix} j' & \lambda & j \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}, \quad (6.3A.13)$$

and

$$\langle I'\|Y^{\lambda}\|I\rangle = (-1)^{I'}\frac{\hat{I}\hat{I}'\hat{\lambda}}{(4\pi)^{\frac{1}{2}}}\begin{pmatrix} I' & \lambda & I \\ 0 & 0 & 0\end{pmatrix}. \quad (6.3A.14)$$

Finally, substitution of the last couple of equations in eq. (6.3A.11) gives

$$(\text{M.E.}) = (-1)^{2I'+J+l+l'+\frac{1}{2}}\left(\frac{2\lambda+1}{4\pi}\right)\hat{I}\hat{I}'\hat{j}\hat{j}'\tfrac{1}{2}\left[1+(-1)^{l'+l+\lambda}\right]$$

$$\begin{Bmatrix} j' & I' & J \\ I & j & \lambda\end{Bmatrix}\begin{pmatrix} j' & \lambda & j \\ \frac{1}{2} & 0 & -\frac{1}{2}\end{pmatrix}\begin{pmatrix} I' & \lambda & I \\ 0 & 0 & 0\end{pmatrix}, \quad (6.3A.15)$$

which leads to eq. (6.3A.19) when substituted in eq. (6.3A.8).

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The Road goes ever on and on
Down from the door where it began.
Now far ahead the Road has gone,
And I must follow, if I can,
Pursuing it with eager feet,
Until it joins some larger way
Where many paths and errands meet.
And whither then? I cannot say.

[The Lord of the Rings,
by J.R.R. Tolkien]

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